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Gava Zang, Zanjan, Iran

Solving Partial Differential Equations with Uncertainties Using Neural-Networks

Applied Mathematics - Numerical Analysis
Master's Thesis

Sajed Zarrinpour Nashroudkoli

Supervisor: Khadije Nedaiasl

Advisor: Parvin Razzaghi

Department of Mathematics

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Abstract

Towards modeling the real-world phenomenons with partial differential equations that involve uncertainties, one of the major difficulties is a set of phenomena known as the curse of dimensionality. Luckily, very often the variability of physical quantities derived from the model can be captured by a few features on the coefficient fields, with what so called model reduction techniques. On the other hand, neural networks are good at finding hidden maps on the data. For example, one can use neural-networks based methods to parametrize the physical quantity of interest as a function of input coefficients. In that case, the representability of such quantity can be justified by viewing the neural networks as performing time evolution to find the solution to the model. Indeed, in this thesis, we review a surrogate forward neural network model used to solve two notable partial differential equations in engineering and physics. Also, we explain possibilities that neural networks comes forward throw looking at the mathematical analysis of a well known method, namely finite element method.

Keywords: *Partial Differential Equations, Finite Difference Method, Finite Element Method, Uncertainty Quantification*

Contents

Chapter 1

Introduction

This chapter begins with introducing the basic concepts required for the rest of the thesis, such as uncertainty quantification and neural networks. It follows by introducing two partial differential equations that we want to solve. This chapter is concluded by an overview of the structure of the thesis.

1.1 Background & Motivation

To model real-world phenomenons, one makes assumptions to simplify his model. More often than not, the hidden parameters that take part in the model are unknown. In many other cases, the exact value of the inputs is unclear. These are examples of what called uncertainty. Usually, one wants to quantify these uncertainties to control them, if possible. Often, models are consist of a single or a system of Partial Differential Equations (PDEs). Then it is beneficial to study methods to solve PDEs that contain uncertainties in their structures. However, incorporating uncertainty would increase both complexity and computational time.

Our interests come from modeling the mechanical behavior of soft tissue, breast in particular, under compression. There are multiple methods to imaging the tissue. For

example, consider magnetic resonance imaging (MRI) and ultra sound (US). Each imaging method uses a different wave length, and because the tissue under study is a composite tissue they will produce different results. This cause a lesion to be identify in one method as healthy and unhealthy in another. On the other hand, each imaging method requires a different patient position. Considering the elasticity of breast, it will deform in any of these positions differently. For example in MRI guided biopsy, the patient is in the prone position and the breast compress via two rigid plate, while in ultra sound the patient is in the supine position and the breast is under no extra pressure than the gravity. This cause the lesion to be identify in potentially different location and size and shape in each image. Then to produce a reliable result, one has to compare/combine the results of these different imaging methods.

Due to its importance in diagnosing and treatment of breast cancer, this problem is an exciting subject for many researchers [1, 2, 3, 4, 5, 6, 7]. For example in [6, 7, 5], finite element method (FEM) is used for modeling. However, according to [7] the main problem with FEM is it's long computation time. They tried to use a machine learning FEM based method to solve the issue and they succeed in getting the result in clinical time. However, their model is not patient specific. In the effort to improve their work, we are after answering this question: 'How can we make it both patient-specific and efficient to use in actual clinics?'.

The first challenge is that each body has different properties, e.g., elasticity. To our knowledge, there is no definite way to determine the exact value of these properties yet. Then they can be thought of as uncertain coefficients in the model.

Next challenge is that the results of such modeling must compute in clinical time. This can be addressed with the proper usage of neural networks as illustrated in [7]. Indeed this notion, using neural network for enhancing numerical approximation, is not new [8, 9, 10, 11, 12, 13].Hence, one can consider solving PDEs with uncertainties using neural networks as a key tool in patient specific modeling of the soft tissue deformation.

In this thesis, we are interested in

i. A better understanding of existing numerical methods bottlenecks which cause time consumption,

ii. Studying ways in which one can avoid those bottlenecks,

iii. Applying proposed method on different problems and see how much changes it needs in structure to adapt.

Two PDEs studied to cover both linear (in 1D) and nonlinear (in 2D) cases.
It worth mentioning that the numerical method that generates the dataset for the neural network to learn, has not much of an importance in our study. It is true that the error in the initial dataset may has impact on the final result, but studying error propagation is not in this thesis boarders. Hence, the classic finite difference method (FDM) is used to generate the initial dataset. However, to achieve our first goal, which was to understand the reason behind time consumption of FEM in the breast modeling problem, the analysis of FEM is presented here. It is indeed useful because any other numerical method that has similar bottleneck is also doomed.

1.2 Partial Differential Equations

The idea behind PDE is simple; to describe the variation of a physical quantity that depends on multiple physical variables, one has to find its partial variation with respect to each physical variable while keeping others constant. Then, summing up all the variations shall give the overall variation of that quantity. To write this in math, one needs a mathematical equation that involves those independent variables, the unknown function (which depends on those variables), and partial derivatives of the unknown function with respect to the independent variables which call a PDE. By definition,

the order of a PDE is the order of the highest derivative involved. A solution (or a particular solution) to a PDE then is a function that turns it into an identity when substituted into the equation. A solution is called general if it contains all particular solutions of the equation concerned [14].

PDEs have been used to formulate the solution of physical problems involving functions of several variables mathematically such as the propagation of heat or sound, fluid flow, elasticity, electrostatics, electrodynamics, etc [14].

If all terms of a PDE contain the dependent variable or its partial derivatives, then such a PDE is called inhomogeneous or homogeneous otherwise. The external forces to the PDE models usually apply through the inhomogeneous term.

One needs additional information about the initial state of the model or change of it over the boundary called conditions to find the unique solution of a PDE. There are two types of conditions, initial conditions, and boundary conditions. An initial condition expresses the value of the solution or its derivatives at an initial point in time. A boundary condition, on the other hand, defines the value of the solution or its derivatives at the boundary of the domain of the problem. Boundary conditions often categories into three categories; *Dirichlet* boundary condition defines the value of the exact solution. *Neumann* boundary condition describes the values of the derivatives of the exact solution. Finally, *Robin* boundary condition describes both the solution and the derivatives. Note that the Robin boundary condition can formulate as a linear combination of the Dirichlet and Neumann boundary conditions.

1.3 Uncertainty Quantification

This section gives an overview of an aspect of this work that mentioned in Section (1.1), which is uncertainty quantification (UQ). We talk briefly about the uncertain parameters of our model, and we describe what the model intends to do with them.

UQ is the end to end the study of the reliability of scientific inference that means the study of relationships between pieces of information, not the 'truth' of those information/assumptions [15]. In other words, given information about uncertainties in the input of a PDE, UQ seeks to determine information about the uncertainties in its output [34]. In that regard, one can extract PDE derived physical quantities as functionals of their random coefficient field. This can potentially impose the need to solve the PDE an exponential number of times. Fortunately, often these functionals depend only on a few characteristic 'features' of the coefficient field that can be determined from solving PDE a limited number of times [16].

Uncertainty is either from an inherently variable phenomenon known as 'aleatoric' or emerges from the lack of knowledge known as 'epistemic'. Epistemic uncertainty concerns the correctness of the structure of the model itself while aleatoric uncertainty concerns the correct values of the parameters of the model [15]. It is clear then that in this thesis, uncertainties are assumed to be aleatoric.

There are four major types of uncertain inputs: random parameters, random fields, white noise, and correlated. Random parameters are a finite number of random numbers each may vary independently according to its own given one-dimensional probability distribution function (PDF) or according to a given joint multivariate PDF collected in a vector called a random vector. On the other hand, random fields are defined over the spatial/temporal domain which means they represent values that vary randomly from one point to another and/or from one time instant to another each of which is determined by sampling from a single PDF (they are identically distributed). In the case of white noise in addition to being identically distributed, the value of the field at a point x and time t is independent of its value at all other spatial points and time instants (they are independent and identically distributed (i.i.d.) and hence uncorrelated). Finally, colored or correlated random fields are identically but not independently distributed [34]. In this thesis, the uncertain inputs are considered to be random parameters and

white noise respectively for our first and second problems.

Often, the output(s) obtained by post-processing the solution of the PDE is more interesting than the solution of the PDE itself. Hence, one can say that provided enough information about the uncertainty in the inputs of the PDE, a UQ task is to determine information about the uncertainty in the output of interest that depends on the solution of a PDE [34].

In our first case, as discussed in Section (3.1), after solving the PDE, a post-processing procedure will apply to obtain an effective coefficient in the media. In the second case, the value of having a surrogate model is more significant due to the nonlinear cubic term, which makes it more difficult to solve numerically. In this case, we are interested in the smallest eigenvalue of the equation.

Assuming random inputs parameterized by the random parameters $\boldsymbol{a} = (a_1, \ldots, a_N)^T$, the solution of the PDE is not only a function of spatial position $\boldsymbol{x}$ and/or time t, but also a function of the random parameter vector $\boldsymbol{a}$. Then, a realization of a solution $u(x, t; a)$ of a PDE is a solution obtained for a specific choice for the random parameters. However, there is no interest in individual realizations in general [34]. This is a hint on how we are going to create the datasets to train and test our model. As we mentioned earlier, the determination of the quantity of interest (which can be either the output of interest derived from the solution of the PDE through some post-processing or the solution of the PDE depend on the situation), often requires the evolution of a multidimensional integral for parameters $a_1, \ldots, a_N$. Quadrature rules are used to approximate such integrals since usually they cannot be evaluated exactly [34]. Our model encapsulates the evolution and do its approximation at the same time. To get a glimpse of the idea, consider that instead of using methods that require the evolution of the quantity of interest for many choices of the parameter vector they depend on to determine statistical information, one can use relatively few solutions of the PDE to build a surrogate model, e.g. an interpolant or a reduced order model, for either

the PDE itself or for the quantity of interest derived from the PDE. Indeed, the model constructed in this thesis is a surrogate model which is a map from the coefficient field $\mathscr{A}$ to the solution space. If the reader is more interested in solving PDE directly with a neural network, we refer him/her to the deep Ritz method (DRM) which uses the self-adjoint problem [17] and the physical informed neural networks (PINN) which tend to create constraints derived directly from the PDE itself in the form of its loss function [18, 19]. There is a tiny note to mention here, that though our examples are elliptic PDEs our model can be used for any type of PDE since it is a surrogate model.

1.4 Artificial Neural Network

In 1943, Warren McCulloch and Walter Pitts [20] wrote a paper on how neurons might work. They modeled a simple neural network with electrical circuits. Although the study of the human brain is thousands of years old, this was the beginning of a new field that evolve into what we know today as artificial neural networks (ANN).
The short history of the development of deep neural networks goes as follow. "In the late 1940s, D.O. Hebb created a learning hypothesis that became known as Hebbian learning [21]. The first functional networks with many layers called 'Group Method of Data Handling' were created by Ivakhnenko and Lapa in 1965 [22, 23, 24]. The basics of continuous backpropagation [22, 25, 26] were derived in the context of control theory by Kelley [27] in 1960 and by Bryson in 1961, using principles of dynamic programming [28]. In 1970, Seppo Linnainmaa published the general method for automatic differentiation (AD) of discrete connected networks of nested differentiable functions [29, 30]. Geoffrey Hinton et al. (2006) proposed learning a high-level representation using successive layers of binary or real-valued latent variables with a restricted Boltzmann machine [31] to model each layer. In 2012, Ng and Dean created a network that learned to recognize higher level concepts, such as cats, only from watching unlabeled images [32].

Unsupervised pre-training and increased computing power from graphics processing units (GPU) and distributed computing allowed the use of larger networks, particularly in the image and visual recognition problems, which became known as "deep learning". Neural Networks, as we know them today, are network or circuit of real biological neurons or their artificial counterparts. In the latter case, we call it artificial neural network. In this thesis, we are working strictly on ANN and we might use the term neural network (NN) for simplicity.

ANNs are composed of artificial neurons that hold the biological concept of neurons that are receiving input, combine it with their internal state and turn on or off. They do that using weights, bias and activation function.

The weights have used to model the connections of the biological neurons. A **weight** is a 'parameter' associated with a connection from one neuron M, to another neuron N. It corresponds to a synapse in a biological neuron, and determines how much notice the neuron N pays to the activation it receives from neuron M [33].

In 'feedforward' and some other neural networks, each hidden unit, and each output unit is connected via a trainable weight to a unit (the **bias** unit) that always has an activation level of 1. This gives a trainable threshold equal to the value of the weight from the bias unit to each hidden or output unit [33]. Moreover, **activation function** is the function that describes the output of a neuron. Most network architecture starts by computing the weighted sum of the inputs. The total net input, is then usually transformed in some way, using activation function. The simplest activation function is a step function; If the total net input is less than 0 (or more generally, less than some threshold T) then the output of the neuron is 0, otherwise, it is 1. A common activation function is a logistic function [33]. The important characteristic of the activation function is that it provides a smooth, differentiable transition as input values change, i.e. small changes in input would produce small changes in output.

Mathematically, we can model a neuron as

$$\psi(XW + b). \tag{1.1}$$

Here, X is the input vector, W is the weight matrix, b is the bias and finally, ψ is the activation function. With this notation, the final output of our feedforward network would be

$$\Phi(X, W^1, \ldots, W^K) = \psi_k(\psi_{k-1}(\ldots \psi_2(\psi_1(XW^1+b^1)W^2+b^2)\ldots W^{K-1}+b^{K-1})W^K+b^K). \tag{1.2}$$

The initial input of the ANN is external data, such as images and documents. The ultimate output is to accomplish a task, such as recognizing an object within the image. To accomplish the task, the neural network would go through a process that we call learning. There are two general types of learning; learning from the data associated with labels which is called supervised learning and learning from unlabeled data which is called unsupervised learning. In this thesis, we would do supervised learning.
Learning, in case of supervised learning, is to minimize a function like $\mathscr{L}(Y, \Phi(X, W^1, \ldots, W^K))$ (i.e. **loss** function e.g. mean square error) that defines a relation between the network output $\Phi(X, W^1, \ldots, W^K)$ and the expected network output Y, which is the labels associated with the data

$$\min_{\{W^k\}_{k=1}^K} \mathscr{L}(Y, \Phi(X, W^1, \ldots, W^K)). \tag{1.3}$$

If the network were unable to minimize the loss function, we say that **underfitting** happened. To ensure that the network learned correctly, we have to test it against a fresh dataset which it hasn't see before, which called the test dataset. What we expect is an acceptable result from our network over this dataset concerning some metrics (e.g mean absolute error). If those results were satisfying, we say that the network learned

successfully. If not, we would say that **overfitting** happened. It means that though the network has perfect results on the training dataset itself, it was unable to generalize the hidden relation of the training dataset (i.e. the provided data set in learning phase) to the test dataset.

The learning process begins by feeding a **batch** of train data to the network. The network try to adjust it's weights so that it minimizes loss function. Then next batch will feed the network. Each passes through all of the train data is called an **epoch**. The whole learning process would often consist of many epochs. But one must be careful about overfitting the data with too many epochs.

There are two different choices to generate data sets when dealing with PDEs. First, solve the PDE over a bigger mesh to obtain the train data set and then solving the PDE over a finer mesh to generate test dataset. Second, picking a percentage of the data points concerning normal distribution over the domain. Moreover, to approach the problem, methods can be categorized into three categories. First, we know the PDE and its coefficients. What we seek is to solve the PDE directly using neural networks. In that regard, one may use the Ritz variational formulation of the PDE to define the loss function and uses the stochastic gradient decent (SGD) optimization algorithm as the optimizer. This way, a numerical approximation of the solution can be calculated much like any other numerical methods [17], or else, one may use a coarse grid to train the network and then use the trained model on a fine grid mesh [35]. Second, the PDE is known but the coefficients are unknown [18, 16]. Finally, neither PDE nor it's coefficients are known [19].

Consider some PDEs with the random coefficient field, we are interested in finding our physical quantities as functionals which depend only on a few characteristic "features" of the coefficient fields through our neural network. A dimension reduction technique based on neural network representation has used to do regression.

Regression seeks to find a function h_θ parameterized by a parameter vector $\theta \in \mathbb{R}^p$ such

that

$$f(\theta) \approx h_\theta(a), a \in \mathbb{R}^q \tag{1.4}$$

For example in linear regression, we need to handcraft a set of basis $\{\phi_k(a)\}$ such that $f(a) = \sum_k \beta_k \phi_k(a)$. However, this process exposes us to the risk of overfitting. A key advantage of the neural network is that it does not need a set of handcrafted basis functions; it bypasses that with learning a direct approximation of $f(a)$ that satisfies (1.4) in a data driven way.

More precisely, we want to learn $f(a)$ that maps the random coefficient vector a in a PDE to some physical quantities described by the PDE.

The approach is conceptually simple, consisting of the following steps

i. Sample the random coefficients (a in (1.4)) of the PDE from a user-specified distribution. For each set of coefficients, solve the deterministic PDE to obtain the physical quantity of interest ($f(a)$ in (1.4)),

ii. Use a neural network as the surrogate model $h_\theta(a)$ in (1.4) and train it using the previously obtained samples,

iii. Validate the surrogate forward model with more samples.

We note that our work is a report of [16]. In this thesis, the function that we want to parameterize is over the coefficient field of the PDE. Now, back to the questions which this thesis is based upon. 'Why one may interested in solving a PDE, especially in the presence of uncertainty, using neural network, and how?' To highlight the important aspect of the idea of using a neural network for solving PDEs, consider these questions. Would it be nice if we can solve our problem on a bigger mesh to train our network and then use it to compute the solution over a finer mesh? How about solving problems with high dimensions in which the classical numerical methods such as FEM and FDM suffer the curse of dimensionality? As we will see in the next section, computing the

basis function over nodal points is the source of heavy computational cost in FEM. What if we would be able to bypass the need to compute them? These are just some of the applications which one may find when importing neural network as a tool in numerical analysis.

1.5 An Overview of Classical Numerical Methods

One of the popular numerical method for solving PDEs is Finite Difference Method (FDM). It is based on the idea of substituting the derivatives in the equation with their approximations. To do so, one may define a mesh, write down the value of each partial derivative on each nodal point of the mesh, and then calculating a numerical approximation for the solution of the partial differential equation. The precision of the method has a direct relation with the order of the precision which we chose to approximate the derivatives in and it can be computed through the Taylor expansion. Though the FDM is a good method and it is widely used, it has its downsides too. An important one is that the FDM cannot be used on complex domains [36, 37, 38].

Finite Element Method (FEM) is based on the variational formulation of the equation and uses more complex mesh structures and it is utilized to investigate problems with more complex domains. One can either use **Ritz** formulation which writes an equivalent minimization problem or **Galerkin** formulation which uses the basics of integration by part and Green's identities to reduce the order of the differential equation. Either way, one would write an equivalent problem to the desired differential equation using basis functions. After achieving the variational formulation, one would approximate its solution by reducing the infinite dimension of the solution space to a finite dimension. Hence, the method is called **finite element method** [39, 40].

Although FEM is very popular, it cannot be used for high dimensional problems referred

in literature as *the curse of dimensionality*. Moreover, refinement of the mesh would result in increasing the nodal points count which means an increase in computational cost. Finally, FEM can explore more domains, yet the domain has to be Lipschitz. We would study finite element method in more details in Section (2.2) [41, 42].
For the enthusiastic reader, here is a list of some other numerical methods: wavelet method [43, 44], finite volume method [45, 46] and meshfree method [47, 48].

1.6 Problem Statement and Contributions

As we saw in Section (1.2), PDEs come to life to express the relations between changing quantities. In this section, we discuss a bit about the problems which we want to solve. Suppose we have inhomogeneous media (inhomogeneous media are media in which all properties of interest are not the same at any point). Also, suppose that we have different values for conductance for different materials, which composed our media, modeled by $a(x)$. Given the fixed direction vector $\xi \in \mathbb{R}^d$, we are interested to know the effective conductance through the media in that direction. More precisely, we want to find the solution to the following minimization problem

$$A_{\text{eff}}(a) = \min_{u(x)} \int_{[0,1]^d} a(x)||\nabla u(x) + \xi||_2^2 \mathrm{d}x. \tag{1.5}$$

For the second problem, we want to know the ground state energy of an electron along with its spatial distribution. Ground state energy is the state which electron wants to be in when the temperature drops to zero. It is equivalent to the smallest eigenvalue of the problem of the form

$$Hu = Eu, \tag{1.6}$$

which in case of multi electrons, is

$$Eu(r) := [-\Delta + v(r) + \int w(r - r^*)|u(r^*)^2|dr^*]u(r). \tag{1.7}$$

In (1.6), H is a Hamiltonian operator which is the sum of the kinetic energies of all the particles, plus the potential energy of the particles associated with the system. Considering multiple particles, our second equation

$$-\Delta u(x) + a(x)u(x) + \sigma u(x)^3 = E_0 u(x),\ x \in [0,1]^d,\ s.t. \int_{[0,1]^d} u(x)^2 \mathrm{d}x = 1, \tag{1.8}$$

can be derived from (1.6). In (1.8), $-\Delta u(x)$ represents the kinetic energy, $a(x)$ is the potential.

The main contributions of this work are:

i. Explaining the bottleneck of the existing numerical methods which led to high computational cost.

ii. Constructing a simple neural network with regular activation and loss functions to approximate the function of interest $f(a)$.

iii. Studying the effectiveness of the network on both linear (in 1D) and nonlinear (in 2D) cases.

1.7 Thesis Structure

The rest of this thesis is structured as follows. In Chapter 2, the mathematical preliminaries needed to understand the thesis are presented. In Chapter 3, we propose our discretization and neural model for the problems. In Chapter 4 we use the proposed model in Chapter 3 to compute the solution and report the results and conclude.

Chapter 2

Mathematical Preliminaries

In this chapter, the required mathematical background to understand the rest of the thesis has discussed. It begins with functional analysis. It will be use to show the convergence of the NN model. Then, It goes over the mathematics of the FEM to demonstrate the necessity of developing new methods that can perform better than our classical methods. This chapter has been concluded by the universal approximation theorem that ensures the existence of a neural network that approximates the solution.

2.1 Functional Analysis

This section begins with introducing measures and follows by Lebesgue integration and functional spaces. This section has been heavily influenced by [15]. Interested readers may go further by reading [15, 49].

2.1.1 Measure Spaces

Sample spaces are abstract sets. One can label certain subsets of these sets with a numerical notion of their 'size' and call them 'measurable'. To be exact

Definition 2.1. A *measurable space* is a pair $(\mathscr{X}, \mathscr{F})$, where

i. $\mathscr{X}$ is a set (the sample space),

ii. $\mathscr{F}$ is a $\sigma - algebra$ on $\mathscr{X}$, (i.e. collection of subsets of $\mathscr{X}$ containing ϕ and closed under applying countable operations of union, intersection, and complementation relative to $\mathscr{X}$).

This, brings up a new definition for the elements of space holding a property.

Definition 2.2. Let $(\mathscr{X}, \mathscr{F}, \mu)$ be a measure space.

i. If $N \subseteq \mathscr{X}$ is a subset of a measurable set $E \in \mathscr{F}$ such that $\mu(E) = 0$, then N is called a μ-null set.

ii. If the set of $x \in \mathscr{X}$ for which some property $P(x)$ does not hold is μ-null, then P is said to hold μ-almost everywhere (or, when μ is a probability measure, μ-almost surely).

Moreover, we need a more precise definition of the notion of integration in this new space.

Definition 2.3. Let $(\mathscr{X}, \mathscr{F})$ and $(\mathscr{Y}, \mathscr{G})$ be measurable spaces. A function $f : \mathscr{X} \to \mathscr{Y}$ generates a $\sigma - algebra$ on $\mathscr{X}$ by

$$\sigma(f) := \sigma([f \in E] | E \in \mathscr{G}),$$

and f is called a *measurable function* if $\sigma(f) \subseteq \mathscr{F}$. That is, f is measurable if the pre-image $f^{-1}(E)$ of every $\mathscr{G}$-measurable subset E of Y is an $\mathscr{F}$-measurable subset of $\mathscr{X}$. A measurable function whose domain is a probability space is usually called a *random variable*.

2.1.2 Lebesgue Integration

The integration of a measurable function with respect to a (signed or non-negative) measure is referred to as *Lebesgue integration*. One can guess that it extends the simple Riemann integral of functions of a single real variable, can handle worse singularities than the Riemann integral.

The Lebesgue integral can define in three steps.

Step i. Calculating Lebesgue integral over simple functions.

Definition 2.4. Let $(\mathscr{X}, \mathscr{F}, \mu)$ be a measure space. The indicator function $\mathbb{I}_E$ of a set $E \in \mathscr{F}$ is the measurable function defined by

$$\mathbb{I}_E := \begin{cases} 1, & \text{if } x \in E \\ 0, & \text{if} x \notin E. \end{cases}$$

A function $f : \mathscr{X} \to \mathbb{K}$ is called simple if

$$f = \sum_{i=1}^{n} \alpha_i \mathbb{I}_{E_i}$$

for some scalars $\alpha_1, \ldots, \alpha_n \in \mathbb{K}$ and some pairwise disjoint measurable sets $E_1, \ldots, E_n \in \mathscr{F}$ with $\mu(E_i)$ finite for $i = 1, \ldots, n$. The Lebesgue integral of a simple function $f := \sum_{i=1}^{n} \alpha_i \mathbb{I}_{E_i}$ is defined to be

$$\int_{\mathscr{X}} f \mathrm{d}\mu := \sum_{i=1}^{n} \alpha_i \mu(E_i).$$

Step ii. Calculating the integral of non-negative measurable functions using simple functions.

Definition 2.5. Let $(\mathscr{X}, \mathscr{F}, \mu)$ be a measure space and let $f : \mathscr{X} \to [0, +\infty]$ be a

measurable function. The Lebesgue integral of f is defined to be

$$\int_{\mathscr{X}} f \mathrm{d}\mu := \sup\left\{ \int_{\mathscr{X}} \phi \mathrm{d}\mu \middle| \begin{array}{l} \phi : \mathscr{X} \to \mathbb{R} \text{ is a simple function, and} \\ 0 \leq \varphi(x) \leq f(x) \text{ for } \mu\text{-almost all } x \in \mathscr{X} \end{array} \right\}$$

Step iii. The integral of a real- or complex-valued function is defined through integration of positive and negative real and imaginary parts, with care being taken to avoid the undefined expression '$\infty - \infty$'

Definition 2.6. Let $(\mathscr{X}, \mathscr{F}, \mu)$ be a measure space and let $f : \mathscr{X} \to \mathbb{R}$ be a measurable function. The Lebesgue integral of f is defined to be

$$\int_{\mathscr{X}} f \mathrm{d}\mu := \int_{\mathscr{X}} f_+ \mathrm{d}\mu + \int_{\mathscr{X}} f_- \mathrm{d}\mu$$

provided that at least one of the integrals on the right-hand side is finite. The integral of a complex-valued measurable function $f : \mathscr{X} \to \mathbb{C}$ is defined to be

$$\int_{\mathscr{X}} f \mathrm{d}\mu := \int_{\mathscr{X}} (\mathrm{Re} f) \mathrm{d}\mu + \int_{\mathscr{X}} (\mathrm{Im} f) \mathrm{d}\mu.$$

It is worthy to define the spaces of Lebesgue integrable functions which are ubiquitous in analysis.

Definition 2.7. Let $(\mathscr{X}, \mathscr{F}, \mu)$ be a measure space. For $1 \leq p \leq \infty$, the L^p space (or Lebesgue space) is defined by

$$L^p(\mathscr{X}, \mu; \mathbb{K}) := \{ f : \mathscr{X} \to \mathbb{K} | f \text{ is measurable and } \|f\|_{L^p(\mu)} \text{ is finite} \}.$$

For $1 \leq p \leq \infty$, the norm is defined by the integral expression

$$\|f\|_{L^p(\mu)} := \left(\int_{\mathscr{X}} |f(x)|^p \mathrm{d}\mu(x) \right)^{1/p}. \tag{2.1}$$

To be more precise, $L^p(\mathscr{X}, \mu; \mathbb{K})$ is the set of equivalence classes of such functions, where functions that differ only on a set of μ-measure zero are identified.

2.1.3 Sobolev Spaces

Definition 2.8. A *multi-index* α is an n-tuple $\alpha = (\alpha_1, \ldots, \alpha_n)$, used to concisely denote the partial differential operator

$$D^\alpha(u) := \frac{\mathrm{d}^{|\alpha|}}{\mathrm{d}x_1^{\alpha_1} \ldots \mathrm{d}_x^{\alpha_n}}(u). \tag{2.2}$$

We define $|\alpha| = \alpha_1 + \cdots + \alpha_n$ to be the *degree* of α.

Definition 2.9. For two multi-indices α, β we define the following:

i. $\alpha \leq \beta$ if $\alpha_i \leq \beta_i$, for all $1 \leq i \leq n$

ii. If $\alpha \leq \beta$, we define $\alpha - \beta := \gamma$, where $\gamma = (\alpha_1 - \beta_1, \ldots, \alpha_n - \beta_n)$

iii. $\alpha! = \alpha_1! \ldots \alpha_n!$

Notation 1. For the remainder of this subsection, let Ω be a bounded open subset of $\mathbb{R}^n$. In general, Ω would be the domain of the PDE which we want to solve.

Definition 2.10. Weak Derivative. Let $\Omega \subset \mathbb{R}^n$, $u, v \in L^p(\Omega)$, and α be a multi-index. Then v is the weak α-th partial derivative of u if

$$\int_\Omega u D^\alpha \phi \mathrm{d}x = (-1)^{|\alpha|} \int_\Omega v \phi \mathrm{d}x$$

for all $\phi \in \mathscr{C}_0^\infty$.

Definition 2.11. Let $1 \leq p \leq \infty$ and k be a non-negative integer. The *Sobolev Space* $\mathscr{W}^{k,p}(\Omega)$ consists of all functions $u : \Omega \to \mathbb{R}, u \in L^p_{loc}(\Omega)$ such that each weak derivative

$D^\alpha u$ with $|\alpha| \leq k$ exists and belongs to L^p. That is,

$$\mathscr{W}^{k,p}(\Omega) = \{u \in L^p_{loc}(\Omega) | \|D^\alpha u\|_{L^p(\Omega)}, \forall |\alpha| \leq k\} \tag{2.3}$$

Similarly, the space $\mathscr{W}^{k,p}_{loc}(\Omega)$ consists of the functions u as above for which $D^\alpha u$ with $|\alpha| \leq k$ exists and belongs to $L^p_{loc}(\mathscr{V})$, where $\mathscr{V}$ is an arbitrary compact subset of Ω.

Remark 2. Note that $\mathscr{W}^{k,p}(\Omega) = \{u \in L^p_\Omega \mid D^\alpha u \in L^p_\Omega, |\alpha| \leq k\}$.

Theorem 2.12. *Assume $u, v \in \mathscr{W}^{k,p}(\Omega)$, $|\alpha| \leq k$. Then*

i. $D^\alpha(\Omega) \in \mathscr{W}^{k-|\alpha|,p}(\Omega)$ and $D^\beta(D^\alpha u) = D^\alpha(D^\beta u) = D^{\alpha+\beta}u$ for all multi-indices α, β satisfying $|\alpha| + |\beta| \leq k$.

ii. For each $\lambda, \mu \in \mathbb{R}$, $\lambda u + \mu v \in \mathscr{W}^{k,p}(\Omega)$ and $D^\alpha(\lambda u + \mu v) = \lambda D^\alpha u + \mu D^\alpha v$, $|\alpha| \leq k$.

Definition 2.13. Norm on $u \in \mathscr{W}^{k,p}(\Omega)$ can be defined by

$$\|u\|_{\mathscr{W}^{k,p}(\Omega)} := \begin{cases} \left(\sum_{|\alpha|\leq k} \int_\Omega |D^\alpha u|^p \mathrm{d}x\right)^{1/p}, & \text{if } 1 \leq p \leq \infty \\ \sum_{|\alpha|\leq k} \operatorname*{ess\,sup}_\Omega |D^\alpha u|, & \text{if} p = \infty. \end{cases}$$

The following theorem states that Sobolev spaces are complete.

Theorem 2.14. *Let $\Omega \in \mathbb{R}^n$ be an open bounded set and $1 \leq p \leq \infty$. Then*

i. the space $\mathscr{W}^{k,p}(\Omega)$ is a Banach space with respect to the norm $\|\cdot\|_{\mathscr{W}^{k,p}}$

ii. the space $H^1(\Omega) := \mathscr{W}^{1,2}(\Omega)$ is a Hilbert space with inner product

$$\langle u, v\rangle := \int_\Omega uv\,dx + \sum_{i=1}^N \int_\Omega \frac{\partial u}{\partial x_i}\frac{\partial v}{\partial x_i}\,dx.$$

Lemma 3. Given $u \in \mathscr{W}^{k,p}(\Omega)$ and $v \in \mathscr{C}^\infty_0(\Omega)$, $uv \in \mathscr{W}^{k,p}(\Omega)$.

Up to this point, the goal was to expand the vocabulary to use it in theoretic justifications of the NN model. Like understanding the universal approximation theorem, or showing the convergence of NN model. Here, it is fit to take a closer look at the FEM, and through that, pin pointing the bottlenecks of it, if any.

2.2 Finite Element Method

This section would review FEM. The goal is to highlight the limitations of this method. For interested readers, we suggest reading FE resources [39, 40]. Moreover, one may be interested in using parallel programming to enhance FEMs performance [50]. However, one needs to question the nature of the method itself to find a way to improve it.

Notation 4. Let Ω be an open set in $\mathbb{R}^n$ and let $k \in \mathbb{N}$. Denote the set of all continuous real-valued functions by $\mathscr{C}^k(\Omega)$. These functions defined on Ω such that $D^\alpha u$ is continuous on Ω for all $\alpha = (\alpha_1, \ldots, \alpha_n)$ with $|\alpha| \leq k$. Assuming that Ω is a bounded open set, $\mathscr{C}^k(\Omega)$ will denote the set of all u in $\mathscr{C}^k(\Omega)$ such that $D^\alpha u$ can be extended from Ω to a continuous function on $\bar{\Omega}$, the closure of the set Ω, for all $\alpha = (\alpha_1, \ldots, \alpha^n)$, $|\alpha| \leq k$. $\mathscr{C}^k(\bar{\Omega})$ can be equipped with the norm

$$\|u\|_{\mathscr{C}^k(\bar{\Omega})} := \sum_{|\alpha| \leq k} \sup_{x \in \Omega} |D^\alpha u(x)|.$$

In particular when $k = 0$ we shall write $\mathscr{C}(\bar{\Omega})$ instead of $\mathscr{C}^0(\bar{\Omega})$ to denote the set of all continuous functions defined on $\bar{\Omega}$; in this case,

$$\|u\|_{\mathscr{C}(\bar{\Omega})} = \sup_{x \in \Omega} |u(x)| = \max_{x \in \bar{\Omega}} |u(x)|.$$

Similarly, if $k = 1$,

$$\|u\|_{\mathscr{C}(\bar{\Omega})} = \sum_{|\alpha|\leq 1} \sup |D^{\alpha}u(x)| = \sup_{x\in\Omega} |u(x)| + \sum_{j=1}^{n} \sup_{x\in\Omega} |\frac{\partial u}{\partial x_j}(x)|.$$

Definition 2.15. The support of a continuous function u on an open set $\Omega \subset \mathbb{R}^n$ is defined as the closure in Ω of the set $x \in \Omega : u(x) \neq 0$. We shall write *supp* u for the support of u, which is the smallest closed subset of Ω such that $u = 0$ in $\Omega \setminus \text{supp } u$.

Denote the set of all u contained in $\mathscr{C}^k(\Omega)$ whose support is a bounded subset of Ω by $\mathscr{C}_0^k(\Omega)$. Let $\mathscr{C}_0^{\infty} = \cap_{k\geq 0}\mathscr{C}_0^k(\Omega)$.

Remark 5. Assuming that the reader is familiar with Hilbert spaces, the Hilbert space $\mathscr{H}_0^1(\Omega)$ has significant importance in our context. It defines as follows:

$$\mathscr{H}_0^1(\Omega) = \left\{ u \in L^2(\Omega) | \frac{\partial u}{\partial x_i} \in L^2(\Omega),\, i = 1, \ldots, n,\, u = 0 \text{ on } \partial\Omega \right\}.$$

2.2.1 Weak Solutions to Elliptic Problems

Let Ω be a bounded open set in $\mathbb{R}^n$, and consider the linear second-order partial differential equation

$$-\sum_{i,j=1}^{n} \frac{\partial}{\partial x_j}\left(a_{i,j}(x)\frac{\partial u}{\partial x_i}\right) + \sum_{i=1}^{n} b_i(X)\frac{\partial u}{\partial x_i} + c(x)u = f(x),\, x \in \Omega \tag{2.4}$$

$$u = 0 \text{ on } \partial\Omega \tag{2.5}$$

where $\partial\Omega$ indicates the boundary of the domain Ω,

$$a_{i,j} \in \mathscr{C}^1(\bar{\Omega}), \quad i,j = 1, \ldots, n; \quad b_i \in \mathscr{C}(\bar{\Omega}), \quad i = 1, \ldots, n; \quad c \in \mathscr{C}(\bar{\Omega}), \quad f \in \mathscr{C}(\bar{\Omega})$$

and

$$\sum_{i,j=1}^{n} a_{i,j}(x)\zeta_i\zeta_j \geq \tilde{c}\sum_{i=1}^{n}\zeta_i^2, \quad \forall\zeta = (\zeta_1,\ldots,\zeta_n) \in \mathbb{R}^n, \quad x \in \bar{\Omega}, \tag{2.6}$$

here $\tilde{c}$ is a positive constant independent of x and ζ. The condition in (2.6) is usually referred to as *uniform ellipticity* and (2.4) is called an elliptic equation. Here, as 2.5 stated, we took the boundary condition as Dirichlet boundary condition for simplicity.

Definition 2.16. A **classical solution** of (2.4) is any function $u \in \mathscr{C}^2(\Omega) \cap \mathscr{C}(\bar{\Omega})$ which satisfies (2.4) and (2.5).

According to the theory of partial differential equations, the equation (2.4) with boundary condition (2.5) has a unique classical solution, provided that $a_{i,j}, b_i, c, f$ and $\partial\Omega$ are sufficiently smooth. In order to overcome the limitations of the classical theory and deal with partial differential equations with non-smooth data, the idea is to generalise the notion of solution by weakening the differentiability requirements on u.

Definition 2.17. Let $a_{i,j} \in L^\infty(\Omega)$, $i,j = 1,\ldots,n$, $b_i \in L^\infty(\Omega)$, $i = 1,\ldots,n, c \in L^\infty(\Omega)$, and let $f \in L^2(\Omega)$. A function $u \in \mathscr{H}_0^1(\Omega)$ satisfying

$$\sum_{i,j=1}^{n}\int_\Omega a_{i,j}(x)\frac{\partial u}{\partial x_i}\frac{\partial v}{\partial x_j}\mathrm{d}x + \sum_{i=1}^{n}\int_\Omega b_i(x)\frac{\partial u}{\partial x_i}v\mathrm{d}x + \int_\Omega c(x)uv\mathrm{d}x = \int_\Omega f(x)v(x)\mathrm{d}x,\ \forall v \in \mathscr{H}_0^1(\Omega) \tag{2.7}$$

is called a **weak solution** of (2.4), (2.5). All partial derivatives in 2.7 should be understood as weak derivatives.

Clearly, if u is a classical solution of (2.4), (2.5), then it is also a weak solution of (2.4), (2.5). However, the converse is not true. If (2.4), 2.5 has a weak solution, this may not be smooth enough to be a classical solution. The first step in the construction of a FEM for an elliptic boundary value problem, (e.g. (2.4), (2.5)) is to convert it into

its weak formulation

$$\text{find } u \in \mathscr{V} \text{ such that } a(u,v) = l(v)\ \forall v \in \mathscr{V}. \tag{P}$$

where $\mathscr{V}$ is the solution space (e.g. $\mathscr{H}_0^1(\Omega)$ for the homogeneous Dirichlet boundary value problem), $a(\cdot,\cdot)$ is a bilinear functional on $\mathscr{V}\times\mathscr{V}$, and $l(\cdot)$ is a linear functional on $\mathscr{V}$. The second step in the construction is to replace $\mathscr{V}$ in (P) with a finite-dimensional subspace $\mathscr{V}_h \subset \mathscr{V}$, which consists of continuous piecewise polynomial functions of a fixed degree associated with a subdivision of the computational domain; then consider the following approximation of (P):

$$\text{find } u_h \in \mathscr{V}_h \text{ such that } a(u_h,v_h) = l(v_h)\ \forall v_h \in \mathscr{V}_h. \tag{P_h}$$

Suppose, for example, that

$$\dim \mathscr{V}_h = N(h) \text{ and } \mathscr{V}_h = \operatorname{span}\{\phi_1,\ldots,\phi_{N(h)}\}$$

where the (linearly independent) basis functions $\phi_i, i = 1,\ldots,N(h)$, have "small" support. Expressing the approximate solution u_h in terms of the basis functions, ϕ_i, we can write

$$u_h(x) = \sum_{i=1}^{N(h)} U_i\phi_i(x), \tag{$\star\star$}$$

where $U_i, i = 1,\ldots,N(h)$, are to be determined. Thus, (P_h) can be written as follows:

$$\text{find } (U_1,\ldots,U_{N(h)}) \in \mathbb{R}^{N(h)} \text{ s.t. } \sum_{i=1}^{N(h)} a(\phi_i,\phi_j)U_i = l(\phi_i),\ j = 1,\ldots,N(h). \tag{P_h'}$$

This is a system of linear equations for $U = (U_1,\ldots,U_{N(h)})^T$, with the matrix of the system $A = (a(\phi_i,\phi_j))$ of size $N(h)\times N(h)$. Because the ϕ_i's have small support,

$a(\phi_i, \phi_j) = 0$ for most pairs of i and j, so the matrix A is sparse (in the sense that most of its entries are equal to 0); this property is crucial from the point of efficient solution - in particular, fast iterative methods are available for sparse linear systems. Once $(P_h{}')$ has been solved for $U = (U_1, \ldots, U_{N(h)})^T$, the expansion $(\star\star)$ provides the required approximation to u. The matrix A is called the stiffness matrix. It is clear that to solve the PDE, one has to construct this stiffness matrix, which in turns impose the necessity of calculating basis functions $\phi_i, i = 1, \ldots, N(h)$ on nodal points. Thus, time needed to computations grows as the number of the nodal points grows. In a sense, if one can solve the PDE without the need to compute the basis function values over nodal point, he can improve computational cost.

2.2.2 The Self-Adjoint Elliptic Problem

In the special case, when the boundary value problem is self-adjoint, i.e.,

$$a_{i,j} = a_{j,i},\ i, j = 1, \ldots, n,\ x \in \bar{\Omega},$$

and

$$b_i \equiv 0,\ i = 1, \ldots, n,\ x \in \bar{\Omega},$$

the bilinear functional $a(\cdot, \cdot)$ is symmetric in the sense that

$$a(v, w) = a(w, v), \quad \forall v, w \in \mathscr{H}_0^1(\Omega).$$

Thus, consider

$$-\sum_{i,j=1}^{n} \frac{\partial}{\partial x_j}\left(a_{i,j}(x)\frac{\partial u}{\partial x_i}\right) + c(x)u = f(x),\ x \in \Omega u = 0 \text{ on } \partial\Omega \tag{2.8}$$

with $a_{i,j}(x)$ satisfying the ellipticity condition (2.6); $a_{i,j} = a_{j,i}$, $c(x) \geq 0$, $x \in \bar{\Omega}$. If we define the quadratic functional $J : \mathscr{H}_0^1(\Omega) \to \mathbb{R}$ by

$$J(v) = \frac{1}{2}a(v, v) - l(v),\ v \in \mathscr{H}_0^1(\Omega).$$

then we can restate (2.8) as a minimization problem.

Lemma 6. Let $u \in \mathscr{H}_0^1(\Omega)$ be the (unique) weak solution to (P) with $\mathscr{V} = \mathscr{H}_0^1(\Omega)$ and suppose that $a(\cdot, \cdot)$ is a symmetric bilinear functional on $\mathscr{H}_0^1(\Omega)$; then u is the unique minimizer of $J(\cdot)$ over $\mathscr{H}_0^1(\Omega)$.

Lemma 7. Let $u \in \mathscr{H}_0^1(\Omega)$ minimizes $J(\cdot)$ over $\mathscr{H}_0^1(\Omega)$; then u is the (unique) solution of the problem (P) with $\mathscr{V} = \mathscr{H}_0^1(\Omega)$. The problem (P) is called the **Euler-Lagrange equation** for this minimization problem.

As we would see in (2.18), convexity is very important in our context. Indeed, it is easy to show that $J(\cdot)$ is convex, i.e.

$$J((1-\theta)v + \theta w) \leq (1-\theta)J(v) + \theta J(w),\ \forall \theta \in [0, 1], \quad \forall v, w \in \mathscr{H}_0^1(\Omega),$$

which follows from the identity

$$(1-\theta)J(v) + \theta J(w) = J((1-\theta)v + \theta w) + \frac{1}{2}\theta(1-\theta)a(v-w, v-w)$$

and the fact that $a(v-w, v-w) \geq 0$. Also, note that if u minimises $J(\cdot)$ then $J(\cdot)$ has a stationary point at u.

One can see that following problems are equivalent:

$$\text{find } u \in \mathscr{H}_0^1(\Omega) \text{ such that } a(u, v) = l(v)\ \forall v \in \mathscr{H}_0^1(\Omega), \tag{W}$$

$$\text{find } u \in \mathscr{H}_0^1(\Omega) \text{ such that } J(u) \leq J(v)\ \forall v \in \mathscr{H}_0^1(\Omega). \tag{M}$$

Given that $\mathscr{V}$ is a certain finite-dimensional subspace of $\mathscr{H}_0^1(\Omega)$ which consists of continuous piecewise polynomiyals of a fixed degree, then the finite element approximation of (W) and (M) would be as follows respectively:

$$\text{find } u_h \in \mathscr{V}_h \text{ such that } a(u_h, v_h) = l(v_h) \ \forall v_h \in \mathscr{V}_h, \tag{W_h}$$

$$\text{find } u_h \in \mathscr{V}_h \text{ such that } J(u_h) \leq J(v_h) \ \forall v_h \in \mathscr{V}_h. \tag{M_h}$$

The problem of calculating basis functions over nodal points stays still. For enthusiastic readers, it is worth mentioning that the self adjoint elliptic problem, can be used as base for a NN model called Deep Ritz Method [17].

2.3 Neural Network

Before going any further, one has to show that the NN models can do approximation. Universal approximation theorem is the main tool for construction of neural networks which can be used to solve PDEs. It gives information needed to ensure that a network would converge to the solution of the problem. It states that a feedforward network with a single hidden layer containing a finite number of neurons can approximate continuous functions on compact subsets of $\mathbb{R}^n$, under mild assumptions on the activation function. George Cybenko in 1989 proved the theorem for *sigmoid* activation functions [51]. Later, in [52] it has been shown that the class of deep neural networks is a universal approximation if and only if the activation function is not polynomial. It had shown in 1991 by Kurt Hornik that it is not the specific choice of the activation function, but rather the multilayer feedforward architecture itself which gives neural networks the potential of being universal approximators [53]; the output units are always assumed to be linear.

feedforward networks with a single hidden layer are universal approximators. However,

the width of such networks has to be exponentially large. In 2017 Lu et al. proved universal approximation theorem for width bounded deep neural networks [54]. In particular, they showed that width $n + 4$ networks with ReLU activation functions can approximate any *Lebesgue integrable function* on n-dimensional input space with respect to L^1 distance if network depth is allowed to grow which can be achieved with *Residual Networks* [55, 56]. They also showed the limited expressive power if the width is less than or equal to n. A later result of their work showed that ReLU networks with width $n + 1$ is sufficient to approximate any continuous function of n-dimensional input variables [57]. We are not going to dive deep in the theory so we refer interested readers to [58, 59] references and we conclude by writing down the theorem itself.

Theorem 2.18. ***(Universal Approximation Theorem)***.

i. ***(Unbounded Width case)*** *Let $\varphi : \mathbb{R} \to \mathbb{R}$ be a non-constant, bounded, and continuous function (called the activation function). Let I_m denote the m-dimensional unit hypercube $[0, 1]^m$. The space of real-valued continuous functions on I_m is denoted by $C(I_m)$. Then, given any $\varepsilon > 0$ and any function $f \in C(I_m)$, there exist an integer N, real constants $v_i, b_i \in \mathbb{R}$ and real vectors $w_i \in \mathbb{R}^m$ for $i = 1, \ldots, N$, such that we may define*

$$F(x) = \sum_{i=1}^{N} v_i \varphi\big(w_i^T x + b_i\big)$$

as an approximate realization of the function f; that is,

$$|F(x) - f(x)| < \varepsilon$$

for all $x \in I_m$. In other words, functions of the form $F(x)$ are dense in $C(I_m)$. This still holds when replacing I_m with any compact subset of $\mathbb{R}^m$.

ii. ***(Bounded Width Case)*** *The universal approximation theorem for width-bounded networks can be expressed mathematically as follows*

For any Lebesgue-integrable function $f : \mathbb{R}^n \to \mathbb{R}$ *and any* $\epsilon > 0$*, there exists a fully-connected ReLU network* $\mathcal{A}$ *with width* $d_m \leq n + 4$*, such that the function* $F_{\mathcal{A}}$ *represented by this network satisfies*

$$\int_{\mathbb{R}^n} |f(x) - F_{\mathcal{A}}(x)| \mathrm{d}x < \epsilon.$$

Here is a list of some of important results and works from literature

i. Multilayer feedforward networks are universal approximators [60].

ii. Neural network with unbounded activation functions is universal approximator [61].

iii. Optimal approximation of piecewise smooth functions using deep ReLU neural networks [62].

iv. On the approximation by neural networks with bounded number of neurons in hidden layers [63].

v. Resnet with one-neuron hidden layers is a universal approximator [56].

Chapter 3

Mathematical Models

In this chapter, we will introduce two PDEs which we want to solve as an example. To maintain generality we choose one linear inhomogeneous elliptic equation which is the effective conductance in a non-homogeneous media, and one nonlinear inhomogeneous Schrödinger equation with random background potential.

3.1 Effective Coefficients for Inhomogeneous Elliptic Equation

Let

$$\mathscr{A} = \{a \in L^\infty([0,1]^d) | \lambda_1 \geq a(x) \geq \lambda_0 > 0\}, \tag{3.1}$$

for some fixed constants λ_0 and λ_1. Then the effective conductance/coefficient in a non-homogeneous media can be expressed as a functional $A_{\text{eff}} : \mathscr{A} \to \mathbb{R}$ defined by

$$A_{\text{eff}}(a) = \min_{u(x)} \int_{[0,1]^d} a(x) ||\nabla u(x) + \xi||_2^2 \, \mathrm{dx}, \tag{3.2}$$

where ξ is a fix direction in $\mathbb{R}^d$ with $||\xi||_2 = 1$ ($||.||_2$ is the Euclidean norm). For $x \in [0,1]^d$ the minimizer $u_a(x)$ of the variational problem (3.2) would satisfy the following elliptic partial differential equation:

$$-\nabla \cdot (a(x)(\nabla u(x) + \xi)) = 0. \tag{3.3}$$

To confirm that (3.3) and (3.2) are equivalent we define $\tilde{J}(\lambda)$ as $\tilde{J}(\lambda) = J(u_a + \lambda\phi)$ where $J(u) = \int_{[0,1]^d} a(x)||\nabla u(x) + \xi||_2^2 \,\mathrm{dx}$ for $\lambda \in \mathbb{R}$ and $\phi \in C_0^\infty([0,1]^d)$. Then

$$\begin{aligned}\tilde{J}(\lambda) &= \int_{[0,1]^d} a(x)||\nabla u_a(x) + \lambda\nabla\phi + \xi||_2^2 \,\mathrm{dx} \\ &= \int_{[0,1]^d} a(x)[< \nabla u_a(x) + \xi, \nabla u_a(x) + \xi > + 2\lambda < \nabla u_a(x) + \xi, \nabla\phi > + \lambda^2 < \nabla\phi, \nabla\phi >] \,\mathrm{dx}\,.\end{aligned} \tag{3.4}$$

The idea is to find the minimum of $\tilde{J}(\lambda)$ using its derivatives because we defined $\tilde{J}(\lambda)$ in a way that it has the same minimum as A_{eff}. Lets calculate the derivative of $\tilde{J}(\lambda)$

$$\tilde{J}'(\lambda) = \int_{[0,1]} a(x)[2 < \nabla u_a(x) + \xi, \nabla\phi > + 2\lambda < \nabla\phi, \nabla\phi >] \,\mathrm{dx}\,. \tag{3.5}$$

Due to the definition of $\tilde{J}'(\lambda)$, one can see that $\tilde{J}'(0) = 0$, so

$$\tilde{J}'(0) = 2\int_{[0,1]} a(x)(\nabla u_a(x) + \xi) \cdot \nabla\phi \,\mathrm{dx} \tag{3.6}$$

$$= 2[a(x)(\nabla u_a(x) + \xi) \cdot \phi - \int_{[0,1]} \nabla \cdot (a(x)(\nabla u_a(x) + \xi)) \cdot \phi \,\mathrm{dx}] \tag{3.7}$$

$$= 0. \tag{3.8}$$

Since ϕ is a compact support function on $[0,1]$, then the $\phi = 0$ out of the boundary

$$\tilde{J}'(0) = \int_{[0,1]} -\nabla \cdot (a(x)(\nabla u_a(x) + \xi)) \cdot \phi \,\mathrm{dx} = 0. \tag{3.9}$$

Furthermore, since $\phi \in c_0^\infty$ then for any $\psi \in L^2([0,1]^d)$ there is a sequence like $\{\phi_i\}_{i=0}^\infty$ which converges to ψ. Putting these together yields
$-\nabla \cdot (a(x)(\nabla u_a(x) + \xi)) \overset{\text{a.e}}{=} 0$.

Notation 8. To simplify finite difference notations in higher dimensions, suppose

i. $\{e_k\}_{k=1}^d$ is the the canonical basis in $\mathbb{R}^d$,

ii. $i \in (i_1, \ldots, i_d) | 1 \leq i_1, \ldots, i_d \leq n$.

Then $u_{i \pm e_k}$ denotes $u_{i_1,\ldots,i_k \pm 1,\ldots,i_d}$.

With this notation, to write the finite difference schema one begins by approximating the first and second derivatives:

$$\frac{\partial}{\partial x_k} a(x) = \frac{a_{i+\frac{1}{2}e_k} - a_{i-\frac{1}{2}e_k}}{h} \tag{3.10}$$

$$\frac{\partial}{\partial x_k} u(x) = \frac{u_{i+e_k} - u_i}{h} \tag{3.11}$$

$$\frac{\partial^2}{\partial x_k^2} u(x) = \frac{u_{i+e_k} - 2u_i + u_{i-e_k}}{h^2} \tag{3.12}$$

where $a_{i+\frac{1}{2}e_k} = \frac{a_{i+e_k} + a_i}{2}$ and $a_{i-\frac{1}{2}e_k} = \frac{a_{i-e_k} + a_i}{2}$. Now Lets rewrite (3.3)

$$\begin{aligned}
-\nabla \cdot (a(x)(\nabla u(x) + \xi)) &= -\nabla \cdot (a(x)\nabla u(x) + a(x)\xi) \\
&= -\nabla a(x) \nabla u(x) - a(x)\nabla^2 u(x) - \nabla a(x)\xi \\
&= -\sum_{k=1}^d \frac{\partial}{\partial x_k} a(x) \frac{\partial}{\partial x_k} u(x) - \sum_{k=1}^d a(x) \frac{\partial^2}{\partial x_k^2} u(x) - \sum_{k=1}^d \frac{\partial}{\partial x_k} a(x) \xi_k \\
&= 0.
\end{aligned}$$

Next, we discretize the domain using a uniform grid with step size $h = \frac{1}{n}$ and grid points denoted by $x_i = i \times h$, where the multi-index $i \in \{(i_1, \cdots, i_d) | 1 \leq i_1, \cdots, i_d \leq n\}$ and then we can discretize the former equatoin:

$$
\begin{aligned}
&-\sum_{k=1}^{d} \frac{a_{i+\frac{1}{2}e_k} - a_{i-\frac{1}{2}e_k}}{h} \cdot \frac{u_{i+e_k} - u_i}{h} - \sum_{k=1}^{d} a_{i-\frac{1}{2}e_k} \frac{u_{i+e_k} - 2u_i + u_{i-e_k}}{h^2} - \sum_{k=1}^{d} \xi_k \frac{a_{i+\frac{1}{2}e_k} - a_{i-\frac{1}{2}e_k}}{h} \\
&= -\sum_{k=1}^{d} \frac{a_{i+\frac{1}{2}e_k} u_{i+e_k} - a_{i+\frac{1}{2}e_k} u_i - a_{i-\frac{1}{2}e_k} u_{i+e_k} + a_{i-\frac{1}{2}e_k} u_i + a_{i-\frac{1}{2}e_k} u_{i+e_k} - 2a_{i-\frac{1}{2}e_k} u_i + a_{i-\frac{1}{2}e_k} u_{i-e_k}}{h^2} \\
&\qquad - \sum_{k=1}^{d} \xi_k \frac{a_{i+\frac{1}{2}e_k} - a_{i-\frac{1}{2}e_k}}{h} \\
&= -\sum_{k=1}^{d} \frac{a_{i+\frac{1}{2}e_k}[u_{i+e_k} - u_i] - a_{i-\frac{1}{2}e_k}[u_i - u_{i-e_k}]}{h^2} - \sum_{k=1}^{d} \xi_k \frac{a_{i+\frac{1}{2}e_k} - a_{i-\frac{1}{2}e_k}}{h} \\
&= \sum_{k=1}^{d} \frac{-a_{i+\frac{1}{2}e_k} u_{i+e_k} + [a_{i+\frac{1}{2}e_k} + a_{i-\frac{1}{2}e_k}] u_i - a_{i-\frac{1}{2}e_k} u_{i-e_k}}{h^2} - \sum_{k=1}^{d} \xi_k \frac{a_{i+\frac{1}{2}e_k} - a_{i-\frac{1}{2}e_k}}{h} = 0.
\end{aligned}
$$

Which can be written as $(L_a U)_i = (b_a)_i$ where

$$
(L_a u)_i := \sum_{k=1}^{d} \frac{-a_{i+\frac{1}{2}e_k} u_{i+e_k} + (a_{i-\frac{1}{2}e_k} + a_{i+\frac{1}{2}e_k}) u_i - a_{i-\frac{1}{2}e_k} u_{i-e_k}}{h^2} \tag{3.13}
$$

$$
(b_a)_i := \sum_{k=1}^{d} \frac{\xi_k (a_{i+\frac{1}{2}e_k} - a_{i-\frac{1}{2}e_k})}{h}. \tag{3.14}
$$

Next, to summarize later in matrix form, consider $d = 1$ (for $d > 1$ the process is the same, only the algorithm in computing coefficients matrix need more explanations which addressed in NLSE section by details). Begin by defining matrices, and set the

boundary condition to Dirichlet boundary condition $u_{|_{\partial\Omega}} = 0$,

$$L_a = \frac{1}{h^2}\begin{bmatrix} a_{1-\frac{1}{2}e_1} + a_{1+\frac{1}{2}e_1} & -a_{1+\frac{1}{2}e_1} & & & & \\ -a_{2-\frac{1}{2}e_1} & a_{2-\frac{1}{2}e_1} + a_{2+\frac{1}{2}e_1} & -a_{2+\frac{1}{2}e_1} & & & \\ & \ddots & \ddots & \ddots & & \\ & & -a_{n-1-\frac{1}{2}e_1} & a_{n-1-\frac{1}{2}e_1} + a_{n-1+\frac{1}{2}e_1} & -a_{n-1+\frac{1}{2}e_1} & \\ & & & -a_{n-\frac{1}{2}e_1} & a_{n-\frac{1}{2}e_1} + a_{n+\frac{1}{2}e_1} & \end{bmatrix}_{n\times n},$$

$$b_a = \frac{1}{h}\begin{bmatrix} \xi_1(a_{1+\frac{1}{2}e_1} - a_{1-\frac{1}{2}e_1}) \\ \xi_1(a_{2+\frac{1}{2}e_1} - a_{2-\frac{1}{2}e_1}) \\ \vdots \\ \xi_1(a_{n+\frac{1}{2}e_1} - a_{n-\frac{1}{2}e_1}) \end{bmatrix}_{n\times 1}, U = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix}_{n\times 1}.$$

Then we can write $L_a U = b_a$. However, our boundary condition is not Dirichlet. To apply periodic boundary condition, one needs to patch some elements to L_a and U as follows

$$L_a^{\text{patched}} = \frac{1}{h^2}\begin{bmatrix} a_{1-\frac{1}{2}e_1} + a_{1+\frac{1}{2}e_1} & -a_{1+\frac{1}{2}e_1} & & & & -a_{1-\frac{1}{2}e_1} \\ & & \ddots & \ddots & \ddots & \\ -a_{n+\frac{1}{2}e_1} & & & -a_{n-\frac{1}{2}e_1} & a_{n-\frac{1}{2}e_1} + a_{n+\frac{1}{2}e_1} & \end{bmatrix}_{n\times n},$$

$$U = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix}_{n\times 1},$$

with $a_{1-\frac{1}{2}e_1} = \frac{a_n + a_1}{2}$ and $a_{n+\frac{1}{2}e_1} = \frac{a_1 + a_n}{2}$. The iterative schema needed to generate the data set with sufficient stopping condition is as follow :

Algorithm 1 Calculate U_a

$U^0 \leftarrow 0$;

while (Stop condition is not satisfied) **do**

Solve $L_a^{\text{patched}} U = b_a$ for U with $U^0 \leftarrow U^i$;

$U^{i+1} \leftarrow U^i$;

end while

$U_a \leftarrow U^i$;

Plugging the u_a obtained from algorithm (1) to

$$A_{\text{eff}}(a) = h^d (u_a^T L_a^{\text{patched}} u_a - 2u_a^T b_a + a^T 1) \tag{3.15}$$

will give us $\mathscr{A}_{\text{eff}}$. To generalize this idea to higher dimensions, one can write L_a^{patched} and U for each dimension, then concatenating L_a^{patched} horizontally and U vertically gives required matrices to proceed with the rest of the algorithm. Note that in this case, for b_a we will compute the sum of b_a's in each dimension. In 1D, since we have the analytic solution for effective conductance as defined in (4.1), then we can write $\mathscr{A}_{ex} - \mathscr{A}_{app} < \epsilon$ where $\mathscr{A}_{app}$ is the approximation which can be obtained via substituting current U^{i+1} in (3.15).

3.1.1 Theoretical Justification of Deep Neural Network Representation

Tough everything we saw shows that we can solve PDEs with neural networks directly, here, our primary goal is not that. Instead, we will prove that we can represent a map from coefficient field to our quantities of interest via convolutional neural networks. In this section, theoretical justification of the validity of the method is presented. Note that this section is a copy of [16], hence we just go over important parts. Proofs and

details can be found in [16].

The main idea is to view the solution u of the PDE as being obtained via time evolution, where each layer of the NN corresponds to the solution at discrete time step. In other words, mapping the input a from the first layer to last layer in the NN resembles the time-evolution of a PDE with discrete time-steps. We focus here on the case of solving elliptic equations with inhomogeneous coefficients. Similar line of reasoning can be used to demonstrate the representability of the ground state-energy E_0 as a function of a using an NN.

Assumption 3.1. Let

$$\mathcal{E}(u;a) := \frac{h^d}{2}(u^T L_a u - 2u^T b_a + a^T 1). \tag{3.16}$$

One can see immediately that $\mathscr{A}_{\text{eff}} = 2\min_{u\in\mathbb{R}^{n^d}} \mathcal{E}(u;a)$.

Due to the variational characterization of (3.16), we can minimize $\mathcal{E}(u;a)$ over the solution space, using steepest decent:

$$u^{m+1} = u^m - \Delta t \frac{\partial \mathcal{E}(u;a)}{\partial u} = u^m - \Delta t(L_a u^m - b_a), \tag{3.17}$$

where Δt is a step size (called learning rate in machine learning context) chosen sufficiently small to ensure decent of the energy. The optimization problem is convex due to the ellipticity assumption of the coefficient field a in (3.1) with Lipshitz continuous gradient (which ensures $u^T L_a u > 0$ except for $u = 1$). Therefore the iterative schema converges to the minimizer with proper choice of the step size for any initial condition. Thus we can choose $u^0 = 0$.

At each step, we need to approximate the map from u^m to u^{m+1} in (3.17) using NN approximation. Hence, the process of time-evolution is similar to applying noisy gradient decent on $\mathcal{E}(u;a)$. More precisely, after performing a step of gradient decent update,

the NN approximation incur noise to the update, i.e.

$$v^0 = u^0 = 0, \quad u^{m+1} = v^m - \Delta t \nabla \mathcal{E}(v^m; a), \quad v^{m+1} = u^{m+1} + \Delta t \gamma^{m+1}. \tag{3.18}$$

Here γ^{m+1} is the error for each layer of the NN in approximating each exact time-evolution iteration u^{m+1}. To be sure, instead of u^m, the object that is evolving in the NN as m changes is v^m.

Assumption 3.2. We assume $a \in \mathscr{A} = a \in \mathbb{R}^n | a_i \in [\lambda_0, \lambda_1], \forall i$ with $\lambda_0 > 0$. Under this assumption $\lambda_a := \|L_a\|_2$ and $\mu_a := \frac{1}{\|L_a^\dagger\|_2}$ satisfy

$$\lambda_a = \mathcal{O}(\lambda_1 h^{d-2}), \quad \mu_a = \Omega(\lambda_0 h^d). \tag{3.19}$$

Here for matrices $\|\cdot\|_2$ denotes the spectral norm, $h = 1/n$.

Assumption 3.3. We assume the NN results an approximation error term γ^{m+1} with properties

$$\left\|\gamma^{m+1}\right\|_2 \leq c \|\nabla \mathcal{E}(v^m; a)\|_2, \tag{3.20}$$

$$\mathbf{1}^T \gamma^{m+1} = 0, \tag{3.21}$$

for $m = 0, \ldots, M-1$ when approximating each step of time-evolution.

Lemma 9. The iteration in (3.18) satisfies

$$\mathcal{E}(v^{m+1}; a) - \mathcal{E}(v^m; a) \leq -\frac{\Delta t}{2} \|\nabla \mathcal{E}(v^m; a)\|_2^2, \tag{3.22}$$

and $\Delta t \leq \delta$, $\delta = (1 - \frac{1}{2(1-c)}) \frac{2}{\lambda_a'}$ with $\lambda_a' = (1 + \frac{c^2}{1-c})\lambda_a$. Furthermore,

$$\frac{\Delta t}{2} \sum_{m=0}^{M-1} \left\|\mathcal{E}(v^{m+1}; a)\right\|_2^2 \leq \mathcal{E}(v^0; a) - \mathcal{E}(v^M; a) \leq \mathcal{E}(v^0; a) - \mathcal{E}(u^*). \tag{3.23}$$

Theorem 3.4. *If Δt satisfies the the condition in Lemma 9, given any $\epsilon > 0$, $|\mathcal{E}(v^M; a) - \mathcal{E}(v; a)| \leq \epsilon$ for $M = \mathcal{O}((\frac{\lambda_1^2}{\lambda_0} + \lambda_1)\frac{n^2}{\epsilon})$.*

Theorem (3.4) will immediately results the following theorem:

Theorem 3.5. *Fix an error tolerance $\epsilon > 0$, there exists a neural-network $h_\theta(\cdot)$ with $\mathcal{O}(n^d)$ hidden nodes per-layer and $\mathcal{O}((\frac{\lambda_1}{\lambda_0} + 1)\frac{n^2}{\epsilon})$ layers such that for any $a \in \mathscr{A} = a \in \mathbb{R}^n | a_i \in [\lambda_0, \lambda_1], \forall i$, we have*

$$|h_\theta(a)\mathscr{A}_{\mathit{eff}}(a)| \leq \epsilon\lambda_1.$$

Note that due to the ellipticity assumption $a \in \mathscr{A}$, the effective conductivity is bounded from below by $\mathscr{A}_{\mathit{eff}}(a) \geq \lambda_0 \geq 0$. Therefore the theorem immediately implies a relative error bound

$$\frac{|h_\theta(a) - \mathscr{A}_{\mathit{eff}}(a)|}{\mathscr{A}_{\mathit{eff}}(a)} \leq \epsilon\frac{\lambda_1}{\lambda_0}.$$

3.2 Nonlinear Schrödinger Equation with Inhomogeneous Background Potential

Consider following differential equation:

$$-\Delta u(x) + a(x)u(x) + \sigma u(x)^3 = E_0 u(x), x \in [0,1]^d, s.t. \int_{[0,1]^d} u(x)^2 dx = 1. \tag{3.24}$$

In this eigen value problem, given background potential $a(x)$, we are interested to find the smallest eigen value, *the ground state energy*, E_0. Here, $-\Delta u(x)$ represents the kinetic energy and $\sigma u(x)$ represents interaction between particles of the same kind. Let $\sigma = 2$ and thus, consider a defocusing cubic Schrödinger equation which can be understood as a model for solition in nonlinear photonics or Bose-Einstein condensate

with inhomogeneous media. Similar to the previous section, we would like to solve the discretized version of equation (3.24) as follow

$$(Lu)_i + a_i u_i + \sigma u_i^3 = E_0 u_i, \sum_{i=1}^{n^d} u_i^2 h^d = 1 \tag{3.25}$$

where

$$(lu)_i := \sum_{k=1}^{d} \frac{-u_{i+e_k} + 2u_i - u_{i-e_k}}{h^2}.$$

To solve this equation, we use newton homotopy method as follow. Consider the sequence of NLSE, $\{(Lu)_i + a_i u_i + s u_i^3 = E_0 u_i\}_{i \in \mathbb{I}}$, with the normalization constraint on u, $h^d \langle u_i, u_i \rangle = 1$ with $s = s_1 \dots s_k$ where $0 < s_1 < s_2 < \cdots < s_k = \sigma$. Consider 2D case. When $s = 0$, the coefficient matrix can be calculated as follows:

Algorithm 2 Coefficient matrix

1: $i, j \leftarrow 1$;
2: Devide x_1 to p part and x_2 to q part;
3: **for** $r \in \{1, ..., p * q\}$ **do**
4: **if** $mod(r, q) == 0$ **then**
5: $j = q$;
6: **else**
7: $j = mod(r, q)$;
8: **end if**
9: $i = floor((r - 1)/p) + 1$;
10: **if** $i > p$ **then**
11: $i = mod(i, p)$;
12: **end if**
13: **if** $j > q$ **then**
14: $j = mod(j, q)$;
15: **end if**

if $i == p$ **then**

  $A(r, j) = \frac{1}{h^2}$;

else

  $A(r, ip + j) = \frac{1}{h^2}$;

end if

if $i == 1$ **then**

  $A(r, (p-1)p + j) = \frac{1}{h^2}$;

else

  $A(r, (i-2)p + j) = \frac{1}{h^2}$;

end if

if $j == q$ **then**

  $A(r, (i-1)p + 1) = \frac{1}{h^2}$;

else

  $A(r, (i-1)p + (j+1)) = \frac{1}{h^2}$;

end if

if $j == 1$ **then**

  $A(r, (i-1)p + q) = \frac{1}{h^2}$;

else

  $A(r, (i-1)p + (j-1)) = \frac{1}{h^2}$;

end if

$A(r, r) = -a_{i,j} - \frac{4}{h^2}$;

end for

From algorithm (2), one can find starting values E_0^0 and U^0. Note that, for $s = 0$, it is an standard eigenvalue problem; $AU = E_0 U$. Also,for $s_i > 0$, there is an additional update operation on the diagonal elements, that is, $A(r, r) = A(r, r) + s_i U_{i,j}^2$. Note that the normalization condition had been applied in the method implicitly. Hence, what

the algorithm computes is $E \times h^2$ so there remains another operation $E = E/h^2$. For each S_i, $i > 0$, inverse power method used to solve the NLSE and E_0, V_0 obtained with $s = s_i$ will be used to warm start for the next iteration. The procedure will proceed till $s_k = \sigma$. We used step size equals to 0.4 for that purpose.

In the rest of this thesis, we use algorithm (1) and equation (3.24) as our numerical schema for generating the Data set needed for training and testing the Neural Network that will be discussed in details in next chapter.

Chapter 4

Results

In his chapter, we present the results for the neural schemes.

4.1 Neural Network Architecture

The structure of the network is shown in figure (4-2). The input to the NN is an n^d matrix representing the coefficient field $a \in \mathbb{R}^{n^d}$ on grid points, and the out put of the network will be $\mathscr{A}_{\text{eff}}$. The main part of the network are convolutional layers with ReLU activation function. This extracts the relevant features around each grid points. To incorporate the translational symmetry property of the solution, which is a previous knowledge, one can use a sum-pooling layer followed by a linear map. More precisely, let $d = 2$, $a_{i,j}^{\tau_1\tau_2} := a_{(i+\tau_1)(j+\tau_2)}$ where the additions are done on $\mathbb{Z}_n$. The output of the convolutional layer gives basis functions that satisfy

$$\tilde{\phi}_{k,i,j} = \tilde{\phi}_{k(i-\tau_1)(j-\tau_2)}(a), \qquad k = 1, \dots, \alpha, \quad i, j = 1, \dots, n, \quad \forall \tau_1, \tau_2 = 1, \dots, n.$$

When using the architecture in figure (4-1) for any τ_1, τ_2,

$$\begin{aligned} f(a^{\tau_1\tau_2}) &= \sum_{k=1}^{\alpha} \beta_k \sum_{i,j=1}^{n} \left(\tilde{\phi}_{kij}(a^{\tau_1\tau_2}) \right) \\ &= \sum_{k=1}^{\alpha} \beta_k \sum_{i,j=1}^{n} \left(\tilde{\phi}_{k(i-\tau_1)(j-\tau_2)}(a) \right) \\ &= \sum_{k=1}^{\alpha} \beta_k \phi_k(a), \\ \phi_k &:= \sum_{i,j=1}^{n} \tilde{\phi}_k ij, \end{aligned}$$

where β_k's are the weights of the last densely connected layer. The summation over i, j comes from the sum-pooling operation. Therefore, the later shows that the translational symmetry of f is preserved.

Note that, due to the periodic boundary condition, the input has to extend periodic too.

We solved 1D effective conductance. In 1D, the effective conductance can be expressed

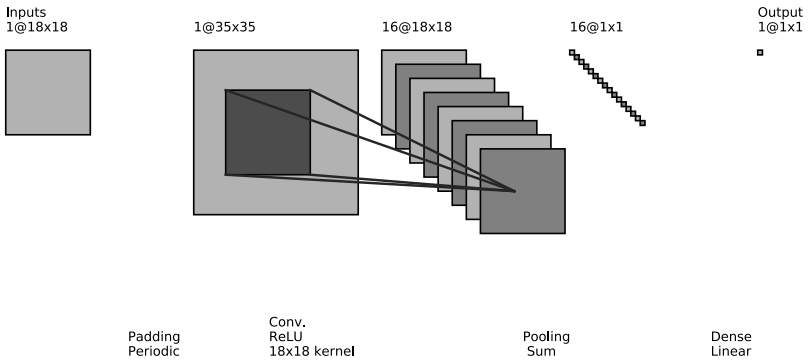

Figure 4-1: Single convolutional layer.

analytically as the harmonic mean of a_i's as follow

$$A_{\text{eff}}(a) = \left(\frac{1}{n}\sum_{i=1}^{n}\frac{1}{a_i}\right)^{-1}. \tag{4.1}$$

Full network schema can be found in figure (4-2). The schema can be divided into three parts. First part is consist of some convolutional layers with size 1 kernel window. Note that the last layer in this part has the channel size 1, since the output of that layer must be a vector of size n. The channel size for the rest of them is chosen to be 16. The plot of the output of this layer can be found in figure (4-3).

Second part is consist of a sum-pooling layer with size n window which produces an scalar.

Although the layers in third part are essentially densely-connected layers, we taken them to be convolutional layers to reflect the symmetry between the first and third parts. Moreover, The input of this part is an scalar.

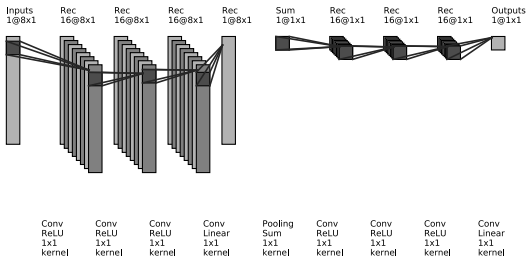

Figure 4-2: Neural network architecture for approximating A_{eff} in 1D.

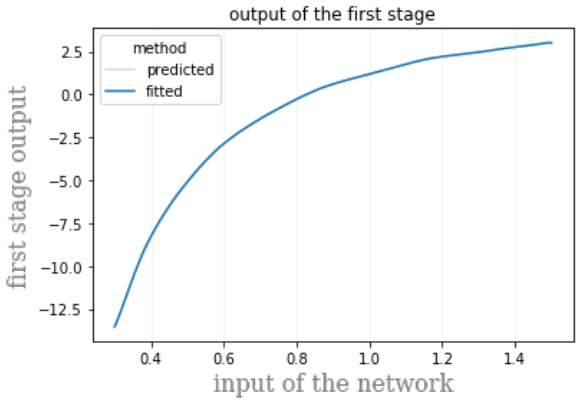

Figure 4-3: Output of the first stage of the neural network in approximating A_{eff} in 1D.

4.2 Effective Conductance in Inhomogeneus Media

We let $d = 1$. We let $a_i \sim \mathscr{U}[0.3, 1.5]$, giving an effective conductance of 0.77 ± 0.13 for $n = 8$. with $\alpha = 16$, we got 2.5793×10^{-5} for the minimum of the loss function (which was mean squared error), and 3.6×10^{-3} for our metric (which was the mean absolute error) on the training set. Moreover, minimum of the loss function on the test set was 5.20×10^{-6} and the metric reported to be 1.74210×10^{-3}. Finally, the predicted effective conductance by the network was 0.76800650 which is acceptable, $\|mean(A_{\text{eff-predicted}}) - mean(A_{\text{eff-exact}})\| = 1.02100 \times 10^{-3}$, and the sum of the error committed over all samples was $\|mean(A_{\text{eff-predicted}} - A_{\text{eff-exact}})\| = 3.4214979 \times 10^{-1}$. More details of the distribution of the error per sample can be found in Figures (4-4) and (4-5).

4.3 Nonlinear Shrödinger Equation

We let $d = 2$, the same network were used except that this time we used a convolutional 2D layer instead of convolutional 1D, and the pooling is also a 2D global pooling layer. 4786 sample were used to train, 861 samples were used to validate, and 1013 sample

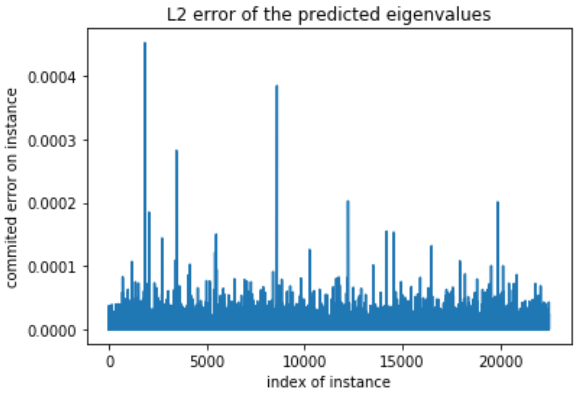

Figure 4-4: Committed error per sample over the prediction set

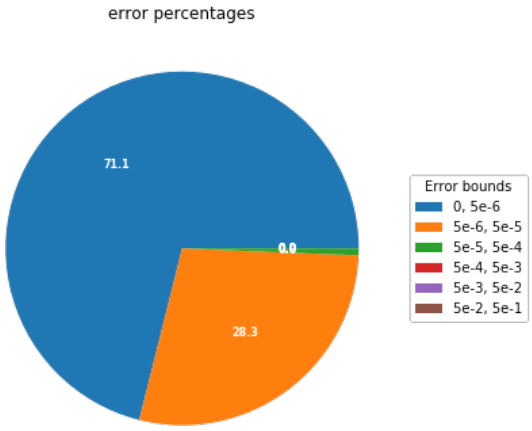

Figure 4-5: Committed error per sample over the prediction set distribution

were used for predictions. Minimum of loss function on the train data, validation data, and prediction sets reported to be 0.0173, 0.0140, and 0.01425044 respectively. Moreover, the metric on those sets reported to be 0.1048, 0.0934, 0.09431260. The mean of predicted ground state had been 10.17474556 which has the L^2-error 7.235×10^{-5} from the mean of the labels, and also is in agreement with the [16]. The number of parameters for our model was 1714, which is higher due to more layer. Figures (4-6) and (4-7) shows more details of committed errors over the prediction set.

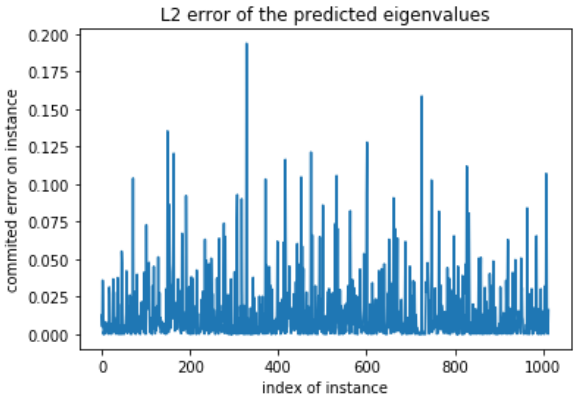

Figure 4-6: Committed error per sample over the prediction set

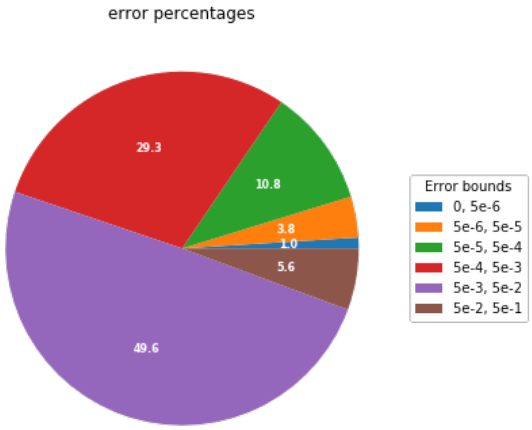

Figure 4-7: Committed error per sample over the prediction set

4.4 Conclusion

We pinpoint the bottle necks of the existed methods. By using neural networks to build a surrogate forward model to solve elliptic partial differential equations. Overall, neural networks seem to be promising for solving partial differential equations.

4.5 Future Work

One of the problems with neural networks is that they have problems with large labels. On the other hands, sometimes, we have large values as the solutions of the PDEs. For example, the ground state energy can be large. We used Z-score normalization. Will this potentially cause error? Is there any better way to deal with these large labels? If not, is there any error bound for this imposed error?

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Chapter 5

Summary of the thesis in Persian

پایگاه داده مستخرج از یک منبع ..... dataset

پایگاه داده مستخرج از منابع متفاوت ..... data set

بیش همسان سازی ..... overfitting

کم همسان سازی ..... underfitting

گشت در داده ها ..... epoch

دسته ..... batch

روش کاهش آشوبناک گرادیان ..... stochastic gradient decent (SGD)

واژه‌نامه فارسی به انگلیسی

شبکه عصبی پیچشی ..... convolutional neural-network

یادگیری عمیق ..... deep learning

روش تفاضلات متناهی ..... finite difference method

روش عناصر متناهی ..... finite element method

محیط ناهمگن ..... inhomogeneous media

شبکه عصبی ..... neural-network

بعد فضائی ..... spatial dimension

عدم قطعیت ..... uncertainty

مقدار سنجی عدم قطعیت ..... uncertainty quantification

غیر خطی ..... nonlinear

مشتق‌گیری اتوماتیک ..... automatic differentiation

هسته پردازنده گرافیکی ..... graphic processor unit (GPU)

شبکه رو به جلو ..... feedforward neural network

شبکه عصبی مصنوعی ..... artificial neural network

بایاس ..... bias

وزن ..... weight

تابع فعال‌سازی ..... activation function

تابع هزینه ..... loss function

نورون ..... neuron

نتیجه‌گیری و کارهای پیش‌رو

همان‌گونه که از نتایج مشهود است، شبکه‌های عصبی توانایی بالایی در تقریب روابط پنهان مابین داده‌ها دارند. همچنین سادگی روش، آن را به یک روش در دسترس تبدیل می‌کند. ضمن اینکه پس از طی مرحله آموزش، شبکه عصبی قادر است جواب مسئله را تقریبا به طور آنی ارائه کند. یکی از محدودیت‌های شبکه‌های عصبی در مورد اندازه مقیاس ورودی‌ها است. به این معنی که در صورتی که برچسب‌ها بسیار بزرگ باشند یا با فاصله بسیار از هم، روند یادگیری با مشکل مواجه می‌شود. همان‌گونه که مشاهده می‌شود خطا در معادله شرودینگر به علت بزرگ بودن برچسب ها در مقایسه با ضرایب عدم قطعیت بیشتر است. ما از روش نرمال سازی Z-Score برای نرمال‌سازی استفاده نمودیم.

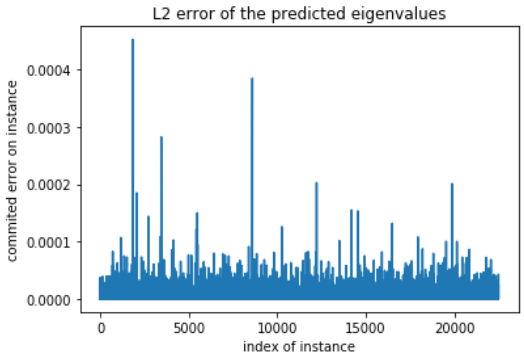
در ادامه این پایان نامه، سؤالات زیر می‌تواند مورد بررسی بیشتر قرار گیرد

- چه روش‌های دیگری برای حل این مسئله موجود است؟
- آیا این نرمال سازی خود خطایی به مدل تحمیل می‌کند؟ کران این خطای تحمیلی چیست؟
- میزان حساسیت شبکه عصبی به خطا در داده‌های ورودی و همچنین الگوی انتشار خطا در آن به چه صورت است؟
- آیا این انتشار خطا با افزایش عمق شبکه و یا استفاده از ساختار های متفاوت اعم از توابع متفاوت برای توابع فعالسازی و همچنین نوع آرایش نورون ها ارتباطی دارد؟

از یک روش تکراری برای حل معادله هستیم. روش حل ما بر مبنای روش هموتوپی نیوتنی بوده است. همچنین دقت شبکه عصبی در معادله شرودینگر به مراتب کمتر از معادله ضریب رسانایی مؤثر است. دلیل این امر را می‌توان به دوعامل نسبت داد. عامل اول تعداد کمتر نمونه‌هاست که به آن اشاره شد و دلیل دوم، بزرگ بودن برچسب ها و کوچک بودن مقیاس فواصل آن‌هانسبت به اندازه خود برچسب‌ها. بهر روی، برای تعدیل این مشکل و بالا بردن دقت داده‌ها توسط روش نرمال‌سازی Z-Score نرمال شده‌اند.

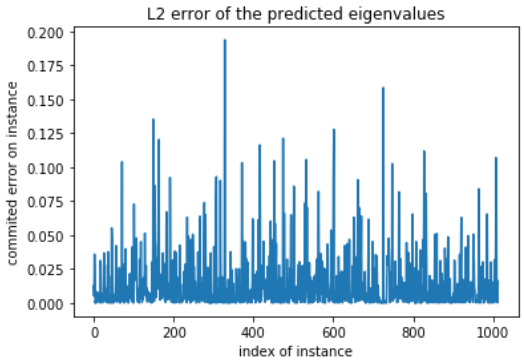
نتایج

مقادیر ضریب رسانایی مؤثر و انرژی حالت پایه به ترتیب ۰٫۷۶۸۰۰۶۵۰ و ۱۰٫۱۷۴۷۴۵۵۶ بدست آمده اند که خطای L^2 به ترتیب، عبارت اند از $۱٫۰۲۱۰۰ \times ۱۰^{-۳}$ و $۷٫۲۳۵ \times ۱۰^{-۵}$. نمودار توزیع خطا بر حسب نمونه برای ضریب رسانایی مؤثر به شرح زیر است.



شکل ۱: خطای مرتکب شده روی مجموعه آزمون به تفکیک نمونه

همچنین، نمودار مشابه برای انرژی حالت پایه نیز به شرح زیر است. همانگونه که مشاهده می‌شود،



شکل ۲: خطای مرتکب شده روی مجموعه آزمون به تفکیک نمونه

تعداد نمونه‌های مورد استفاده قرا گرفته برای آموزش ماشین در معادله شرودینگر بسیار کمتر از معادله ضریب رسانایی مؤثر است. دلیل این امر هزینه بالای محاسباتی برای محاسبات این معادله نسبت به معادله اول بوده است. دقت کنید که در این معادله، به دلیل وجود جمله غیر خطی، مجبور به استفاده

برای حل معادلات با روش تفاضلات متناهی، معادله تعیین ضریب رسانش مؤثر روی یک شبکه نه نقطه‌ای متساوی‌الفاصله، با مقادیر ضرایب عدم قطعیت با توزیع نرمال $\mathcal{U}[۰٫۳, ۱٫۵]$، و معادله شرودینگر غیر خطی روی یک شبکه هشتاد و یک نقطه‌ای متساوی‌الفاصله (گسسته سازی نه نقطه‌ای هر کدام از ابعاد)با مقادیر ضرایب عدم قطعیت با توزیع نرمال $\mathcal{U}[۱, ۱۶]$ به تعداد نمونه‌های مورد نیاز حل می‌شوند. سپس درصدی از تکرارها (در اینجا هفتاد و پنج درصد) به عنوان داده برای مرحله آموزش و الباقی برای مرحله آزمون کنار گذاشته می‌شوند.

شبکه عصبی متشکل از سه بخش است. بخش اول و سوم قرینه یکدیگر و متشکل از لایه‌های پیچشی [1] هستند که به واسطه بخش دوم که یک استخر مجموع [2] است به هم متصل شده‌اند. ورودی این شبکه برای رسانایی مؤثر یک بردار و برای معادله شرودینگر یک ماتریس است. دقت شود که در حالت دو بعدی، قبل از لایه‌های پیچشی، ابعاد داده ورودی گسترش می‌یابد. این امر با توجه به اینکه شرط مرزی مسئله دوره‌ای است، به صورت گسترش دوره‌ای انجام می‌شود. خروجی شبکه در هر دو حالت یک اسکالر است. که در مورد ضریب رسانائی مؤثر، این اسکالر برابر ضریب رسانائی مؤثر در جهت ثابت ξ و در مورد معادله شرودینگر، برابر با سطح انرژی حالت پایه است.

شبکه پس از چندین بار مرور داده‌ها در انتها ضرایب خود را به گونه ای تنظیم می‌کند که تابع هدفی که به آن معرفی کرده‌ایم را کمینه نماید. وقتی تابع مذکور به میزان کمینه خود برسد می‌گوییم آموزش شبکه به اتمام رسیده است. از این پس می‌توانیم با خوراندن ورودی جدید به شبکه از آن برای یافتن جواب استفاده نماییم.

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1 convolutional layers
2 sum-pooling

هر $\epsilon > 0$ یک شبکه ReLu[1] کامل $\mathcal{A}$ با عرض $d_m \leq n + 4$، به گونه ای موجود است که $F_{\mathcal{A}}$ نمایش داده شده با این شبکه در رابطه

$$\int_{\mathbb{R}^n} |f(x) - F_{\mathcal{A}}(x)| \, \mathrm{d}x < \epsilon$$

صدق نماید.

روش پیشنهادی

معادله تعیین ضریب رسانش مؤثر تنها در یک بعد، و معادله شرودینگر در دو بعد حل خواهند شد. هدف این انتخاب تأکید بر این نکته بوده است که با اندک تغییری در ساختار ورودی‌های شبکه، می‌توان از این مدل برای حل معادلات دیفرانسیل در هر بعد دلخواهی استفاده کرد. دلیل این امر نیز استفاده از محاسبات تنسوری در ساختار شبکه عصبی می‌باشد.

توجه خواننده را به این نکته جلب می‌نمائیم که روش عددی‌ای که برای ساخت پایگاه داده اولیه مورد نیاز برای شبکه عصبی استفاده می‌شود، از جهتی حائز اهمیت است؛ زیرا به میزانی که خطای ما روی داده اولیه کمتر باشد اطمینان ما از جواب شبکه عصبی بیشتر است. از طرفی، بررسی اینکه این خطا در داده‌های اولیه چگونه در شبکه عصبی منتشر می‌شود و شبکه تا چه میزان به خطا در داده های ورودی خود حساس است، از حیطه این پایان نامه خارج است. بنابراین، از آنجایی که شبکه عصبی صرفا از یک جدول داده بهره می‌برد و نسبت به اینکه این جدول داده‌ای از چه راهی بدست آمده اطلاع قبلی ندارد، در این پایان نامه فرض بر این است که روش عددی استفاده شده برای ایجاد پایگاه داده با شبکه عصبی غیر مرتبط است و بنابراین از هر روش عددی‌ای می‌توان استفاده نمود. به همین منظور از روش تفاضلات متناهی برای تولید پایگاه داده در هر دو مسئله استفاده نموده‌ایم.

[1] Rectified linear unit

نظارت[1] به عنوان معیاری برای تعیین انحراف جواب‌های شبکه از جواب‌های واقعی معرفی شده به شبکه است. در این صورت، می‌توان روند یادگیری یک شبکه عصبی را معادل با یک مسئله کمینه‌سازی برای کمینه کردن میزان این تابع هدف در نظر گرفت. ابزار شبکه برای کمینه سازی این تابع هدف، تغییر وزن‌ها و بایاس‌های نورون‌های خود است. قضیه زیر که به قضیه تقریب جهانی مشهور است، شرایط استفاده از شبکه‌های عصبی برای تقریب جواب مسئله را بیان می‌کند.

قضیه. (قضیه تقریب جهانی)

۱. **(حالت نامتناهی)** فرض کنید $\varphi : \mathbb{R} \to \mathbb{R}$ یک تابع غیرثابت پیوسته بی‌کران باشد که آن را تابع فعال‌سازی می‌نامیم. فرض کنید I_m بیانگر ابر مکعب mـ بعدی $[۰, ۱]^m$ باشد، و فضای توابع پیوسته حقیقی مقدار روی I_m با $C(I_m)$ نمایش داده شود. در این‌صورت، به ازای هر $\varepsilon > ۰$ دلخواه و هرتابع $f \in C(I_m)$، ثوابت حقیقی مانند $v_i, b_i \in \mathbb{R}$ و بردارهای $w_i \in \mathbb{R}^m$ برای $i = ۱, \ldots, N$وجود دارند، به طوری‌که می‌توانیم

$$F(x) = \sum_{i=۱}^{N} v_i \varphi\left(w_i^T x + b_i\right)$$

را به عنوان تقریبی از f ارائه دهیم:

$$|F(x) - f(x)| < \varepsilon$$

که در آن $x \in I_m$ است. به عبارت دیگر، توابع به شکل $F(x)$ در $C(I_m)$ چگال‌اند.
این نتیجه به ازای هر زیر مجموعه فشرده دیگری از $\mathbb{R}^m$ به جای I_m نیز برقرار است.

۲. **(حالت کران‌دار)** در شبکه‌های کران‌دار، برای هرتابع انتگرال‌پذیر لبگ مانند $f : \mathbb{R}^n \to \mathbb{R}$ و

[1] Supervised learning

تعریف می‌شود. هدف در حل این مسئله یافتن کوچکترین مقدار ویژه آن (حالت پایه) است

$$-\Delta u(x) + a(x)u(x) + \sigma u(x)^{۳} = E_{۰} u(x)$$
$$x \in [۰, ۱]^d, s.t. \int_{[۰,۱]^d} u(x)^{۲} dx = ۱.$$

مشابه آنچه در قسمت قبل آمد معادله فوق را گسسته می‌کنیم

$$(Lu)_i + a_i u_i + \sigma u_i^{۳} = E_{۰} u_i, \sum_{i=۱}^{n^d} u_i^{۲} h^d = ۱ \qquad (۶)$$

که در آن

$$(lu)_i := \sum_{k=۱}^{d} \frac{-u_{i+e_k} + ۲u_i - u_{i-e_k}}{h^{۲}}.$$

شبکه‌های عصبی

شبکه عصبی[۱] از تعدادی واحد متصل به هم نام نورون [۲] تشکیل می‌شود. هر نورون دارای یک وضعیت داخلی است که در ترکیب با داده ورودی تغییر می‌کند و توسط تابع فعال‌سازی[۳] خروجی نورون را به حالت روشن یا خاموش تغیر می‌دهد. به عبارت ریاضی، هر نورون دارای اسکالرهای داخلی به نام وزن[۴] و بایاس[۵] و تابع فعالسازی‌ای است که به ترتیب با W و b و ϕ نمایش داده می‌شوند. و خروجی نورون در این صورت با فرض اینکه X ورودی نورون باشد به صورت $\phi(WX + b)$ خواهد بود. برای این ساختار تابعی به عنوان تابع انحراف[۶] به عنوان تابع هدف تعریف می‌شود که در حالت یادگیری تحت

[1] Neural network
[2] Neuron
[3] Activation function
[4] Weight
[5] Bias
[6] Loss function

با تعاریف بالا جواب را به صورت $L_a U = b_a$ می‌توان نوشت. اما برای رسیدن به گسسته‌سازی نهایی، هنوز نیاز داریم که مسئبه را با در نظر گرفتن شرط مرزی دوره‌ای بازنویسی نماییم.

$$L_a^{\text{patched}} = \frac{1}{h^2} \begin{bmatrix} a_{1-\frac{1}{2}e_1} + a_{1+\frac{1}{2}e_1} & -a_{1+\frac{1}{2}e_1} & & & -a_{1-\frac{1}{2}e_1} \\ & \ddots & \ddots & \ddots & \\ -a_{n+\frac{1}{2}e_1} & & & -a_{n-\frac{1}{2}e_1} & a_{n-\frac{1}{2}e_1} + a_{n+\frac{1}{2}e_1} \end{bmatrix}_{n\times n},$$

$$U = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix}_{n\times 1},$$

که در آن $a_{1-\frac{1}{2}e_1} = \frac{a_n+a_1}{2}$ و $a_{n+\frac{1}{2}e_1} = \frac{a_1+a_n}{2}$. نهایتا پس از حل مسئله توسط یک روش تکراری با گسسته سازی مطرح شده، جواب بدست آمده را در رابطه زیر قرار می‌دهیم تا به رسانایی مؤثر دست یابیم

$$A_{\text{eff}}(a) = h^d(u_a^T L_a^{\text{patched}} u_a - 2u_a^T b_a + a^T 1). \tag{5}$$

تعیین سطح انرژی حالت پایه با پتانسیل زمینه ناهمگون

معادله دوم، معادله غیرخطی شرودینگر دو بعدی است. هدف از این معادله، یافتن میزان انرژی حالت پایه الکترون با پتانسیل اولیه همراه با عدم قطعیت است. حالت پایه سطح انرژی‌ای است که الکترون مایل به اخذ آن در دمای صفر مطلق می‌باشد. این معادله به صورت یک مسئله مقدار ویژه به فرم زیر

که می‌تواند به صورت $(L_aU)_i = (b_a)_i$ نمایش داده شود که در آن

$$(L_au)_i := \sum_{k=1}^{d} \frac{-a_{i+\frac{1}{2}e_k}u_{i+e_k} + (a_{i-\frac{1}{2}e_k} + a_{i+\frac{1}{2}e_k})u_i - a_{i-\frac{1}{2}e_k}u_{i-e_k}}{h^2} \qquad (3)$$

$$(b_a)_i := \sum_{k=1}^{d} \frac{\xi_k(a_{i+\frac{1}{2}e_k} - a_{i-\frac{1}{2}e_k})}{h}. \qquad (4)$$

همان‌طور که اشاره کردیم، قصد ما حل این مسئله در حالت یک بعدی است. بنابراین در روابط بالا $d = 1$ قرار می‌دهیم. با درنظر گرفتن شرط مرزی $u_{|\partial\Omega} = 0$، در مرحله بعد اقدام به نوشتن فرم ماتریسی آن می‌نماییم.

$$L_a = \frac{1}{h^2}\begin{bmatrix} a_{1-\frac{1}{2}e_1} + a_{1+\frac{1}{2}e_1} & -a_{1+\frac{1}{2}e_1} & & & \\ -a_{2-\frac{1}{2}e_1} & a_{2-\frac{1}{2}e_1} + a_{2+\frac{1}{2}e_1} & -a_{2+\frac{1}{2}e_1} & & \\ & \ddots & \ddots & \ddots & \\ & & -a_{n-1-\frac{1}{2}e_1} & a_{n-1-\frac{1}{2}e_1} + a_{n-1+\frac{1}{2}e_1} & -a_{n-1+\frac{1}{2}e_1} \\ & & & -a_{n-\frac{1}{2}e_1} & a_{n-\frac{1}{2}e_1} + a_{n+\frac{1}{2}e_1} \end{bmatrix}_{n\times n},$$

$$b_a = \frac{1}{h}\begin{bmatrix} \xi_1(a_{1+\frac{1}{2}e_1} - a_{1-\frac{1}{2}e_1}) \\ \xi_1(a_{2+\frac{1}{2}e_1} - a_{2-\frac{1}{2}e_1}) \\ \vdots \\ \xi_1(a_{n+\frac{1}{2}e_1} - a_{n-\frac{1}{2}e_1}) \end{bmatrix}_{n\times 1}, U = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix}_{n\times 1}.$$

که در آن $\lambda_۰$ و $\lambda_۱$ اعداد ثابتی هستند.با فرض انتخاب یک جهت دلخواه ثابت $\xi \in \mathbb{R}^d$، میزان ضریب رسانش در آن جهت مطلوب است. به عبارت دقیق‌تر، جواب معادله زیر مد نظر است

$$A_{\text{eff}}(\boldsymbol{a}) = \min_{u(x)} \int_{[۰,۱]^d} \boldsymbol{a}(x)||\nabla u(x) + \xi||_۲^۲ \mathrm{d}x.$$

این معادله با فرم دیفرانسیلی زیر هم‌ارز است. به عبارت دیگر، جواب مسئله بهنه‌سازی فوق در معادله دیفرانسل زیر سدق میکند و جواب معادله دیفرانسیل زیر نیز تابع هدف مسئله بهینه‌سازی فوق را بهینه می‌کند.

$$-\nabla \cdot (a(x)(\nabla u(x) + \xi)) = ۰ \qquad (۲)$$

ازاین‌رو، با جای حل مسئله مینیم‌سازی، فرم مذکور را به کمک گسسته‌سازی زیر با گام $h = \frac{۱}{n}$ حل می‌نماییم.

$$\begin{aligned}
&-\sum_{k=۱}^{d} \frac{a_{i+\frac{۱}{۲}e_k} - a_{i-\frac{۱}{۲}e_k}}{h} \cdot \frac{u_{i+e_k} - u_i}{h} - \sum_{k=۱}^{d} a_{i-\frac{۱}{۲}e_k} \frac{u_{i+e_k} - ۲u_i + u_{i-e_k}}{h^۲} - \sum_{k=۱}^{d} \xi_k \frac{a_{i+\frac{۱}{۲}e_k} - a_{i-\frac{۱}{۲}e_k}}{h} \\
&= -\sum_{k=۱}^{d} \frac{a_{i+\frac{۱}{۲}e_k} u_{i+e_k} - a_{i+\frac{۱}{۲}e_k} u_i - a_{i-\frac{۱}{۲}e_k} u_{i+e_k} + a_{i-\frac{۱}{۲}e_k} u_i + a_{i-\frac{۱}{۲}e_k} u_{i+e_k} - ۲a_{i-\frac{۱}{۲}e_k} u_i + a_{i-\frac{۱}{۲}e_k} u_{i-e_k}}{h^۲} \\
&\qquad - \sum_{k=۱}^{d} \xi_k \frac{a_{i+\frac{۱}{۲}e_k} - a_{i-\frac{۱}{۲}e_k}}{h} \\
&= -\sum_{k=۱}^{d} \frac{a_{i+\frac{۱}{۲}e_k}[u_{i+e_k} - u_i] - a_{i-\frac{۱}{۲}e_k}[u_i - u_{i-e_k}]}{h^۲} - \sum_{k=۱}^{d} \xi_k \frac{a_{i+\frac{۱}{۲}e_k} - a_{i-\frac{۱}{۲}e_k}}{h} \\
&= \sum_{k=۱}^{d} \frac{-a_{i+\frac{۱}{۲}e_k} u_{i+e_k} + [a_{i+\frac{۱}{۲}e_k} + a_{i-\frac{۱}{۲}e_k}] u_i - a_{i-\frac{۱}{۲}e_k} u_{i-e_k}}{h^۲} - \sum_{k=۱}^{d} \xi_k \frac{a_{i+\frac{۱}{۲}e_k} - a_{i-\frac{۱}{۲}e_k}}{h} = ۰.
\end{aligned}$$

مدل مطرح شده در این پایان‌نامه، این تکامل و تقریب عددی جواب آن را به طور همزمان بر عهده دارد. بدین منظور، به جای تلاش برای یافت جواب مدل، در سدد یافت نگاشتی از پارامترهای تصادفی ورودی به خروجی پردازش شده مدل هستیم. دقت کنید که به همین دلیل، با اینکه ما روش خود را روی معادلات بیضوی بررسی کردیم، همین روش برای معادلات هذلولوی و سهموی نیز کاراست.

تعریف مسئله

در این پایان نامه، هدف ما بررسی یک مدل میانبر برای حل مسائل معادلات دیفرانسیل با مشتقات جزئی به کمک شبکه‌های عصبی است. به عبارت روشن‌تر یافتن نگاشتی از فضای عدم قطعیت مسئله به فضای جواب. مسائلی که در این رساله برای حل انتخاب شده اند از این جهت حائز اهمیت بوده‌اند که هر دو حالت خطی و غیر خطی، معادلات دیفرانسیل غیر همگن شامل عدم قطعیت را پوشش می‌دهند.

یافتن ضریب رسانایی مؤثر در محیط ناهمگون

معادله اول، رسانایی مؤثر در یک جهت انتخاب شده درون یک محیط غیر همگون را توسط ضریب رسانش توصیف می‌کند. محیط غیر همگون، محیطی است که در آن خصوصیات مورد توجه در تمامی نقاط یکسان نیستد. این امر ممکن است به دلایلی همچون جنس‌های گوناگون مواد تشکیل دهنده یا چگالی های متفاوت مربوط باشد. فرض ما بر آن است که ضریب رسانایی ماده در جهات متفاوت یکسان نباشد و این ضریب را با $\boldsymbol{a}(x)$ نمایش می‌دهیم. این بردار از نمونه‌گیری توابعی به فرم زیر روی نقاط رأسی حاصل می‌شود:

$$\mathscr{A} = \{a \in L^{\infty}([۰, ۱]^d) | \lambda_۱ \geq a(x) \geq \lambda_۰ > ۰\}, \qquad (۱)$$

مقدارسنجی عدم قطعیت

مقدارسنجی عدم قطعیت مطالعه اعتمادپذیری نتیجه‌گیری علمی است. به عبارت دیگر به جای مطالعه درستی هر فرضیه به طور جزئی، به دنبال مطالعه ارتباط بین فرضیات هستیم. سؤال اساسی در مسائل مقدار سنجی عدم قطعیت این است که با فرض اینکه اطلاعاتی درمورد خطا در ورودی‌های مدل در دسترس باشد، در مورد تغییرات در خروجی چه می‌توان گفت؟(۱۵) برای مقدار سنجی عدم قطعیت یک کمیت فیزیکی، یکی از راه‌ها پیدا کردن نگاشتی از فضای پارامترهای عدم قطعی در ورودی مدل به فضای خروجی مدل است. خوشبختانه این نگاشت‌ها عموما وابسته به تعداد محدودی 'خصیصه' هستند که می‌توان آنها را با تعداد محدودی نمونه‌برداری و حل مدل دیفرانسیلی به‌دست آورد.

عموما عدم قطیت ناشی از فرضیات ساختار مدل و یا مقدار وردی‌های آن است. در این پایان‌نامه، ما روی عدم قطعیت حاصل از عدم قطعیت روی ورودی‌های مدل تمرکز خواهیم کرد. عدم قطعیت روی داده‌های ورودی به چهاردسته پارامترهای تصادفی، میدان‌های تصادفی، نویز سفید و همبسته طبقه‌بندی می‌شود (۱۶). در مسئله یافتن ضریب رسانایی مؤثر پر محیط ناهمگون عدم قطعیت روی داده های ورودی از نوع پارامترهای تصادفی و در مسئله تعیین سطح انرژی حالت پایه با پتانسیل زمینه ناهمگون از نوع نویز سفید هستند.

اغلب مقدار خروجی مورد نظر ما مقداری است که از فراوری داده‌های خروجی مدل اولیه حاصل می‌شود. دراین‌جا نیز، هدف ما در واقع کنترل عدم قطعیت خروجی ثانویه مدل است که از فراوری حاصل می‌شود. با فرض اینکه عدم قطعیت ورودی مدل با بردار $\boldsymbol{a} = (a_1, \ldots, a_N)^T$ پارامتری شده باشد، جواب معادله علاوه بر ابعاد فضایی $\boldsymbol{x}$ و بعد زمان $\boldsymbol{t}$ به بردار پارامترهای رندوم $\boldsymbol{a}$ نیز وابسته است. بنابراین یک نمونه‌گیری از جواب می‌تواند به صورت $u(x,t;a)$ به ازای یک انتخاب مشخص از پارامترهای رندوم بیان شود. گرچه ما علاقه‌مند به بررسی هر کدام از این نمونه‌ها به طور مجزا نیستیم (۱۶). بنابراین ما پایگاه داده خود را بر همین اساس خواهیم ساخت. کنترل عدم قطعیت مقدار خروجی مطلوب معمولا مستلزم تکامل یک انتگرال چندگانه روی بردار پارامتری $\boldsymbol{a}$ است (۱۶).

است که به صورت یک ترکیب خطی از پایه های آن فضا در نقاط رأسی بدست می‌آید. دقت این تقریب با تعداد نقاط رأسی به کار رفته رابطه مستقیم دارد. بنابراین، محاسبه تقریبی دقیق برای مسائل پیچیده روی دامنه‌های پیچیده، همچون محاسبه میزان تغییر فرم بافت پستان در اثر نیروهای وارده، به ناچار مستلزم استفاده از تعداد بسیار زیادی نقاط رأسی روی دامنه مدل می‌باشد که به طور مستقیم منجر به افزایش زمان محاسبه جواب مدل می‌شود. از این‌رو با تکیه بر اصول شبکه‌های عصبی بدنبال راهی برای حذف نیاز به محاسبه مستقیم پایه‌های فضای تقریب روی نقاط رأسی با استفاده از روشی مبتنی بر کاهش بعد فضای جواب با حفظ خصوصیات اصلی مورد نیاز خود از جواب هستیم. با توجه به اینکه نمایش جواب بدست آمده از شبکه‌های عصبی به صورت ترکیبی متناهی از توابع است، می‌توانیم با تعویض نمایش جواب از حالت خطی (روش‌های عددی متداول) با حالت غیر خطی (نمایش شبکه‌های عصبی) به این مهم دست یابیم. ایده، استفاده از شبکه‌های عصبی برای یادگیری نگاشتی از دامنه ضرایب عدم قطعیت به فضای جواب بر اساس مجموعه داده از قبل محاسبه شده است. به این ترتیب می‌توان گفت روشی که ما در صدد گزارش آن هستیم، یک روش کاهش بعد برای محاسبه جواب بدون نیاز به حل مستقیم معادله دیفرانسیل است. در این رساله، معادلات دیفرانسیل با مشتقات جزئی بیضوی خطی و غیر خطی ناهمگن را مورد بررسی قرار می‌دهیم. نکته حائز اهمیت این است که از آن‌جا که این روش، یک روش مبتنی بر داده است، نوع مدل (بیضوی، هذلولوی و یا سهموی) یا روش عددی استفاده شده برای نمونه‌گیری جواب و ایجاد پایگاه داده جدید، در آن تغییر چشمگیری ایجاد نمی‌نمایند. بنابراین، این روش برای هر سه نوع معادلات دیفرانسیل با مشتقات جزئی در هردو حالت همگن و ناهمگن قابل استفاده است. از طرف دیگر، از آنجا که ما از محاسبات تنسوری در لایه‌های این شبکه بهره می‌بریم، این مدل با کمترین میزان تغییرات قابل استفاده در ابعاد بالاتر نیز است. برای نمایش این ادعا، معادله اول را در یک بعد و معادله دوم را در دو بعد بررسی خواهیم کرد.

و برنامه ریزی درمان می‌شود. در این مرحله، راه‌حلی که به ذهن می‌رسد، ترکیب نتایج حاصل از این روش‌ها برای بالابردن ضریب دقت است؛ لیکن مشکل دیگری مانع این‌کار می‌شود. بافت پستان بسیار کشسان است و به راحتی تغییر فرم می‌دهد. از طرفی در هرکدام از این روش‌ها بیمار به حالت خاصی قرار می‌گیرد که با روش دیگر متفاوت است. به طور مثال، طی MRI بیمار در حالت دمر قرار دارد ولی برای تصویربرداری فراصوت بیمار به پشت می‌خوابد. علاوه‌براین، در روش بایوپسی راهنمایی شده توسط MRI[1] بافت پستان توسط صفحه‌های سخت و غیرقابل انعطافی بی حرکت می‌شوند که منجر به فشرده شدن بافت نیز می‌شود. بنابراین، شکل، اندازه و مکان غده در این تصاویر متفاوت خواهد بود. این امر مقایسه تصاویر را با سختی بسیار همراه می‌کند. علاوه‌براین، برای برنامه‌ریزی پیش از جراحی، پزشک نیاز به دانستن مکان و اندازه دقیق غده دارد. بنابراین، نیاز به توسعه الگوریتم‌های ثبت غیرسخت[2] احساس می‌شود.

روش‌هائی مبتنی بر روش المان‌های متناهی[3] برای حل این مسئله ارائه شده‌اند. اما مشکل عمده این روش‌ها هزینه محاسباتی بالای آنها است. مطابق آن‌چه در (۷) گفته شده است، به طور متوسط اجرای یک شبیه‌سازی صد و بیست دقیقه به طول می‌انجامد که برای مصارف کلینیکی مقرون به صرفه نیست. مارتینز و همکارانش (۷) در سدد ارائه روشی برای کاهش این هزینه محاسباتی با استفاده از شبکه‌های عصبی بودند. گرچه، مدل ارائه شده توسط آنها زمان محاسبات را به طرز چشمگیری کاهش می‌دهد، اما پارامترهای مدل مورد مطالعه آن‌ها ثابت است. به عبارت دیگر، با توجه به این‌که این پارامترها از بدنی به بدن دیگر متفاوت هستند، برای ارائه یک مدل مختص به بیمار در زمانی قابل قبول، نیاز به توسعه مدل برای فراگیری پارامترهای دارای عدم قطعیت است. به طور مثال، نیازمند در نظر گرفتن ضریب کشسانی بدن بیمار، که یک ضریب عدم قطعیت است، هستیم. از این رو، برآن شدیم که بدنبال حل عددی معادلات دیفرانسیل (بیضوی) به کمک شبکه‌های عصبی باشیم.

در روش‌های عددی متدوال، هدف یافتن تقریبی از جواب مدل در یک فضای متناهی یا غیر متناهی

[1] MRI-guided biopsy
[2] Non-rigid registration algorithm
[3] Finite element method

جواب معادله است. در این پایان‌نامه تابع مورد نظر برای پارامتری‌سازی روی میدان ضرایب معادله دیفرانسیل با مشتقات جزئی تعریف شده است. در واقع ما به دنبال کاهش بعد مبتنی بر نمایش شبکه عصبی برای حل معادلات دیفرانسیل با مشتقات جزئی همراه با عدم قطیت هستیم.

انگیزه و هدف

مدل‌سازی طبیعت همیشه با پارامترهایی همراه است که مقادیر آنها از کنترل ما خارج است. اما عموما ما درباره محدوده تغییرات این پارامترها اطلاعاتی داریم. به معادلاتی که شامل این‌گونه پارامترها هستند، معادلات با ضرایب عدم قطعیت گوییم. به طور مثال، در مورد حرکت نفت در سفره‌های زیر زمینی؛ برای بیان شیوه حرکت مایعات نیاز به دانستن مکان حفره‌ها در بافت سفره زیر زمینی داریم. این امر را می‌توان به صورت رسانایی مؤثر در حضور ناخالصی نیز در نظر گرفت. به عنوان مثالی دیگر، مسئله‌ای را مطرح می‌کنیم که نقطه شروع این رساله بوده است.

برای تشخیص سرطان پستان روش‌های متعددی موجود است. از جمله آن‌ها می‌توان به تصویر برداری پستان با بازتابش اشعه ایکس (XRM)[۱]، تصویربرداری با استفاده از ارتعاشات مغناطیسی (MRI)[۲]، تصویربرداری فراصوت (US)[۳]، توموسنتز دیجیتال (DBT)[۴]، ماموگرافی انتشار پوزیترون (PET)[۵] و توموگرافی فراصوت (UST)[۶] اشاره کرد. هرکدام از این روش‌ها اطلاعات را به طرق مختلفی نمایش می‌دهند، به این معنا که غده‌ای که در یکی از این روش‌ها غیر قابل تشخیص است در روش دیگر قابل تشخیص است؛ غده‌ای که در یک روش بافت مشکوک معرفی می‌شود، در روش دیگر می‌تواند به عنوان غده‌ای سالم و طبیعی معرفی شود. و این موضوع باعث ایجاد مشکلات بسیاری در روند تشخیص

[1] Projection X-ray mammography
[2] Magnetic resonance imaging
[3] Ultra sound
[4] Digital breast tomosynthesis
[5] Positron emission mammography
[6] Ultra sound tomography

مقدمه

مقدارسنجی عدم قطعیت (۱۵) در فیزیک و مهندسی اغلب شامل مطالعه معادلات دیفرانسیل با مشتقات جزئی با میدان ضرایب تصادفی است. برای درک رفتار یک سیستم شامل عدم قطعیت، می‌توان کمیت‌های فیزیکی مشتق شده از معادلات دیفرانسیل توصیف کننده آن سیستم را به عنوان توابعی از میدان ضرایب استخراج کرد. اما حتی با گسسته‌سازی مناسب روی دامنه معادله و برد متغیرهای تصادفی، این کار به طور ضمنی به حل عددی معادله دیفرانسیل با مشتق جزئی به تعداد نمایی می‌انجامد.

یکی از روش‌های متداول برای مقدار سنجی عدم قطعیت، روش نمونه برداری مونته کارلو است. گرچه این روش در بسیاری از موارد کاربردی است اما کمیت اندازه‌گیری شده ذاتاً دارای نویز است. به‌علاوه، این روش قادر به پیدا کردن جواب‌های جدید در صورتی که قبلا نمونه‌گیری نشده باشند، نیست. ما به‌دنبال یافت روشی هستیم که نویز داده‌ها در جواب آن تأثیر چندانی نداشته باشند و همچنین، قادر به ارائه جواب برای حالاتی که قبلا نمونه گیری نشده باشند نیز باشد.

روش گالرکین تصادفی با استفاده چند جمله‌ای‌های آشوب یک جواب تصادفی را روی فضای متغیرهای تصادفی بسط می‌دهد و به این طریق مسئله با بعد بالا را به تعدادی معادله دیفرانسیل با مشتقات جزئی معین تبدیل می‌کند. این گونه روش‌ها به دقت زیادی درباره تعیین توزیع عدم قطعیت نیازمند هستند و از آن‌جا که پایه‌های استفاده شده مستقل از مسئله هستند، وقتی بعد متغیرهای تصادفی بالا باشد هزینه محاسباتی بسیار زیاد خواهد شد. ما به‌دنبال یافتن راهی برای حذف نیاز به محاسبه این پایه‌ها به صورت سنتی هستیم. یکی از اهداف این پایان‌نامه مطالعه نقطه ضعف روش‌های عددی سنتی همانند روش گالرکین تصادفی و روش المان‌های متناهی است. برای این منظور، تئوری روش المان‌های متناهی را مورد مطالعه دقیق‌تر قرار می‌دهیم.

هدف کار ما پارامتری کردن جواب یک معادله دیفرانسیل معین به کمک شبکه‌های عصبی (ساخت نمایشی دیگر برای جواب بر پایه ترکیب توابع) و سپس استفاده از روش‌های بهینه‌سازی برای یافتن

فهرست

چکیده

برای مدل‌سازی پدیده‌های واقعی با معادلات دیفرانسیل با مشتقات جزئی که شامل عدم قطعیت است، یکی از مشکلات وجود مجموعه‌ای از پدیده‌ها است که به عنوان مشکلات ابعاد بالا شناخته می‌شوند. خوشبختانه، اغلب تغییرات متغییرهای مدل می‌توانند توسط تعداد کمی خصوصیات دامنه توسط روش‌های کاهش مدل، ثبت شوند. برای مثال، می‌توان با استفاده از روش‌های مبتنی بر شبکه‌های عصبی متغییرهای مورد نظر را به عنوان تابعی از ضرایب ورودی اندازه‌گیری کرد. در این‌صورت، نمایش پذیری متغیرها توسط چنین شبکه‌ای را می‌توان با دید شبکه عصبی به عنوان یک تحول زمانی برای پیداکردن جواب‌های مدل توجیه کرد. در این پایان نامه، ما یک روش میانبر برای پیدا کردن جواب‌های مدل روی دو معادله دیفرانسیل با مشتقات جزئی معروف در فیزیک و مهندسی را بازبینی مینمائیم. همچنین، ما به سراغ بررسی یک روش عددی سنتی از نظر تئوری خواهیم رفت و از این طریق، احتمالات جدیدی برای استفاده از شبکه‌های عصبی در حل معادلات دیفرانسیل را مطرح خواهیم نمود.

واژه‌های کلیدی: *شبکه‌های عصبی، روش تفاصلات متناهی، روش المان‌های متناهی، معادلات دیفرانسیل با مشتقات جزئی، عدم قطعیت.*

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حل عددي معادلات ديفرانسيل با مشتقات جزئی با ضرايب نامعين به کمک شبکه عصبی

پایان‌نامهٔ کارشناسی ارشد ریاضیات کاربردی ـ آنالیز عددی

ساجد زرین پور نشرودکلی

استاد راهنما: **دکتر خدیجه ندائی اصل**

استاد مشاور: **دکتر پروین رزاقی**

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