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# UNRAVELING THE OPTIMIZATION LANDSCAPE AND TRAINING DYNAMICS OF NEURAL NETWORK SOLVERS FOR PARTIAL DIFFERENTIAL EQUATIONS

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**Abstract**
This research investigates how neural network solvers are used in Partial Differential Equations (PDEs), particularly the insight the optimization landscape can provide into the training of these solvers. We explore the capabilities of several neural network-based techniques for solving different benchmark PDEs. These techniques include, but are not limited to, the Physics-Informed Neural Network (PINN), Deep Ritz, the Deep Galerkin Method, and so on. The findings show how algorithms affect training optimization. Through optimization algorithms like SGD and Adam, the objective of this paper is to take a closer look at the convergence rate and solution accuracy and stability. We will examine the loss surface of a neural network solver through theoretical analysis and experimental work. We will look at the influence of local minima, saddle points, sharp areas, etc. on these solvers. We also investigate how unstable hyperparameters (like learning rate, batch size, and weight initialization) impact solvers. Overall, the results show that Sasha and Adam outperform SGD in speed and accuracy and can be chosen accordingly. This study can improve the efficiency of neural network tools to solve PDEs It gives a look at how work in the future can help improve these tools especially for more challenging, high-dimensional and multi-physics problems.

## INTRODUCTION

Solvers for Partial Differential Equations (PDEs) are important tools in applications of science and engineering, medicine (e.g. fluid dynamics, heat transfer, and structural mechanics). Techniques such as the Finite Element Method (FEM) and the Finite Difference Method (FDM) have been in existence for decades (Burden & Faires, 2011). While they perform efficiently in certain scenarios, their effectiveness weakens when faced with complexity or high-dimensionality problems. In particular, they find irregular geometries and multi-physics problems difficult (Choi, 2019) . Neural networks are deep learning architectures built using vast neural connections or links. The deep structure is responsible for the emergence of characteristics not present in their elementary counterparts. Current deep neural networks are successful when they use weights to enhance performance. However, enable the network to learn complex features.

Physics-Informed Neural Networks or PINNs is an important application of Deep Learning to solve PDEs. The basic idea of PINNs is to inject the PDE into a neural network's loss function such that the solution satisfies the governing equations at all points during a training (Raissi et al., 2019). This new solver doesn't need mesh generation, which is expensive in compute time and has a clumsy setup for standard solvers. The Deep Ritz Method and Deep Galerkin, two other well-known methods, showed up that use variational methods and Galerkin formulations, respectively (E et al.; Sirignano & Spiliopoulos 2018). Turning problems into bits to solve tough PDEs is not required using these ways thus making them effective and flexible for use.

However, despite their potential, there are several issues around optimization and training dynamics that are preventing the use of neural network solvers for PDEs. To be specific, there has not yet been any analysis of the optimization landscape of these neural networks, including loss surfaces, saddle points, existence of local minima, and so on in the case of PDE solvers. These traits are key for determining the convergence and stability of those solvers while training them. The optimization algorithm, neural network architecture, and PDE (Zhang et al., 2019) all influence these characteristics. There has been a lot of work around optimization perspective of deep learning in general (Bengio et al., 2015), but much less in the case of PDE solvers.

The deep learning community is largely using optimization algorithms like Stochastic Gradient Descent (SGD) and Adam. However, the understanding of their impact on the convergence rate and stability of neural network solvers for PDEs is quite limited (Kingma and Ba, 2014). Choosing an optimal algorithm is essential when optimizing PDE problems. Choosing an incorrect optimization algorithm may decrease the efficiency and reliability of the solution. Moreover, this negative effect increase with the dimension and non-linearity (Reddi et al., 2018). To continue, the initialization of the parameters of the neural network and the tuning of the hyperparameters, for the learning rate and size of the batch, affect the performance of the solver (Yao et al., 2020). It is important as improper network initialization and selection of hyperparameters that are wrong can result in a slow solution or a failure to converge.

The way that we sample the data will also affect the dynamics of the training of the neural network solver for PDEs, besides optimization. This includes the collocation points (CPs) and the boundary conditions (BCs). The data in PINNs consists of collocation points where we impose the PDE and the boundary condition that requires the solution to behave in a certain way on the boundary of the domain. The many sampling strategies can impact training by altering the training data distribution and the networks capability of approximating the solution (Wang et al., 2020). A high number of collocation points used at a location may stabilize convergence quickly. But, as density increases, the computational effort increases. Using sparse sampling may lead to slow convergence or inferior accuracy.

Therefore, the key query of this study is how the optimization landscape, training dynamics and sampling strategies interact with and influence the performance of neural network solvers for PDEs. We want to analyze these factors in great detail to develop more efficient and robust neural network based solvers for PDEs. Many people know very

little about this side of optimization dynamics. Hopefully, through the tackling of the current research problems, more trustworthy models will manage to work with complex real-world PDEs.

This study will analyse the optimisation landscape and training dynamics of neural network solvers for partial differential equations (PDEs). We will investigate how SGD and Adam algorithms' convergence or behavior are affected by the use of distinct sampling schemes and loss functions. The aim is to provide some ideas on how one can perturb the optimization landscape in order to obtain better and more stable solvers for difficult PDEs and thus trigger more and more work in this exciting field of computation.

## 2. Literature Review

Neural networks are having increasing success in addressing Partial Differential Equations (PDE) that cannot be accurately solved by existing techniques due to their high dimensionality and non-linearity or complexity of boundary condition. Direct approximation of the solution can be obtained using neural networks, particularly deep learning methods, without discretizing the problem domain. This review discusses literature on neural network solvers for PDEs, complementary optimization problems, and their training dynamics.

### 2.1 Neural Network-Based PDE Solvers.

Physics-Informed Neural Networks, commonly referred to as PINNs (Raissi et al., 2019), are an important development in machine learning. PINNs use the equations of the governing PDEs in the loss function such that the neural network learns the physics of the scene along with the solution. When you put together the conditions and rules of the PDE, and then leave out the generation of the mesh, the appeal of PINNs for the problems in the complex geometries is quite powerful (Raissi et al., 2019). Some other techniques are the Deep Ritz Method (E et al., 2017), Deep Galerkin Method (Sirignano & Spiliopoulos, 2018). The first uses variational principles while the second uses Galerkin formulations in order to write the PDEs as optimization problems for deep learning.

These methods come in handy as they do not discretize the problem domain, a rather expensive and involved thing to do when the dimension of the problem becomes bigger. They use the continuous approximation instead solution by a neural network which can be trained using an approach of gradient-based optimization which aims to minimize the loss function which encodes the PDE and boundary conditions (Wang et al., 2020). These days, the fluid dynamic codes have been modified specifically to get better on their modelling capability with these high order numerical techniques.

### 2.2 Optimization algorithms and their impact.

Solvers based on neural networks have their advantages but optimization is challenging. The optimization landscape features affect both the training process and solver stability. The landscapes of optimizers in neural networks usually contain local minima, saddle points and plateaux. The training process and complete rates are affected by these features. Great question! Here is a 23 word paraphrase for your text: First studies of deep learning optimization showed that saddle points can slow convergence and prevent from reaching global minimum. (Choromanska et al., 2015).

Neural networks have been trained using various optimization algorithms such as SGD, Adam and Adam variants. SDG is a straightforward yet effective method that can be easily utilized to carry out a wide range of machine learning tasks. The addition of the adaptive optimization algorithm known as Adam has aided in speeding up convergence while maintaining the stability of the training (Kingma & Ba, 2014). Nonetheless, it is not well understood how those algorithms impact the performance of neural network solvers for PDEs. Some studies have shown that Adam can outperform SGD in non-convex optimization spaces. For example, the solution of PDEs (Zhang et al., 2020). But this is highly dependent on the PDE, network and hyperparameters (Reddi et al., 2018).

### 2.3 The Loss surface and training dynamics.

Many researchers are studying loss surfaces of neural networks for PDE solvers. As solvers iterate, it is critical that they converge and remain stable over time. The characteristics of the surface getting iterated on may help the solvers with this. It is useful to know if this surface has a local minimum, saddle

point, or is flat. Zhang et al. did work on deep learning optimization in 2019. To begin with, the authors have shown that the loss surface of deep neural networks (DNNs) is non-convex but may have lots of valleys which are hard to optimize. PDEs may suffer severely from this because, in addition to slow convergence, they may become stuck in poor local minimum and yield an inaccurate solution.

Elliptic equations are an example of some PDEs that have a smoother loss landscape which has relatively few saddle points. Thus, standard optimization methods may facilitate the solution of these PDEs. Futhermore, hyperbolic or parabolic PDEs face, however, convergence which refers to gradient loss that has a much more rugged surface and instabilities. To design better solvers based on neural networks, (Lu et, al., 2019) has proposed a number of insights to better understand the relationship between the properties of the PDE and those of its loss surface.

**2.4 Hyperparameters and Initialization Strategies.**

Neural network solvers for partial differential equations (PDEs) are highly sensitive to the initialization of their network parameters and hyperparameters such as the learning rate, batch size, and momentum. If a neural network is not properly initialized, it may have a slower convergence or diverge completely because the network suffers from the vanishing or the exploding gradients. (Glorot et al., 2010). To assist with these issues, novel techniques for weight initialization such as Xavier and He initialization have been proposed (He et al., 2015). But, the best method has been shown to depend on the specific problem and network architecture.

It is essential to properly set the learning rate as it influences the speed and stability of the learning process. If the learning rate is too high, the algorithm might miss the correct answer entirely. But a rate that is too low will get to the answer slowly. Algorithms that adjust the learning rate like Adam (Kingma & Ba, 2014) reduce this phenomenon by modifying the learning rate based on the gradient size. The effect that learning rate and optimization algorithm have on characteristics of the PDE Solution needs further investigation (Yao et al., 2020).

**2.5 Data Sampling and Boundary Conditions.**

When poor data is purposely chosen and the PINNs solver does not manage to learn the ground truth/generating distribution well and/or sufficiently, it is identified as an effective instance of counter-selection. Increased collocation points yield a more accurate solution for a PDE but at increased cost. On the other hand, we can get late convergence and accuracy less solution by using few collocation points.

We refer to these approaches as a framework to understand the impact of the boundary conditions on the neural network's performance. Accurate boundary condition modelling in the loss function improves the accuracy and stability of the solver (Yao et al, 2020). This works especially well for problems with complicated boundary shapes. Also, neural network solvers can handle strange shapes and strategies. So, they can deal with non-uniform grids a feature that makes them superior to normal numerical methods that only work with uniform grids.

**2.6 Validating the Method with Benchmark Problems**

Researchers know that neural network solutions for PDEs work with benchmark problems: many pitches an actual problem to solve. For instance, Raissi et al. (2019) demonstrated that PINNs could solve a class of nonlinear elliptic and parabolic PDEs such as the Poisson and heat equations. In the same vein, E et al. (2017) showed that Deep Ritz Method has the capability of solving variational problems associated with elliptic PDEs. In 2018,in the paper "Deep Galerkin Method for Elliptic Partial Differential Equations," Sirignano and Spiliopoulos introduced the Deep Galerkin Method. Broadly, the Deep Galerkin Method has been used successfully in several cases such as the Burgers' equation, the Black-Scholes equation, etc.

Neural network solvers accomplish great performance on many problems of interest. But, this capability can change based on the selection of the network architecture, optimization algorithm, and training dynamics. Studies compared different methods for solving complex PDEs. Research papers containing the above statement have identified the strengths and weaknesses of different

approaches and suggested a hybrid approach which combines different neural network architectures and optimization strategies (Wang et al., 2020; Lu et al., 2019).

**2.7 Challenges and Future Directions.**

Even though solvers that use neural networks show a lot of promise, there are challenges. The first problem with these solvers is that they are sensitive to their hyperparameters and the optimisation algorithms. So, they have to be tuned to work well and may not be able to scale complex problems. Moreover, as we do not completely understand the optimization landscape and the effect of convergence, further research is necessary for the proposal of more robust training strategies. Neural network solvers still face a challenge extending to more complex PDEs that involve multi-physics.

In future research, adaptive optimization algorithms have the potential to be developed which change their parameters during training. Alternatively, researchers can explore hybrid methods which leverage the best aspects of traditional numerical methods and deep learning. Neural network-based solvers will also benefit from uncertainty quantification and error analysis (Zhang et al., 2020).

**3. Problem Formulation**

This study investigates neural network solvers for the Poisson equation, the heat equation and the Navier-Stokes equations, selected benchmark Partial Differential Equations (PDEs). We come across partial differential equations in engineering and physical sciences as they are applicable in electromagnetism, fluid dynamics and heat transfer. The Poisson's equation is used to model electrostatic and gravitational potential. The heat equation is a fundamental equation for modelling thermal conduction. According to Verma et al. (2017), the equations that govern the motion of fluid substances are called Navier-Stokes equations. The Navier-Stokes equations play a significant role in aerodynamics, meteorology, and engineering fluid dynamics.

Our aim is to improve the neural network solvers for PDEs and create new ones when necessary. The chosen neural networks are based on the Physics-Informed Neural Networks, Deep Ritz and Deep Galerkin Methods. PINNs were introduced by Raissi et al. (2019). The PDE constraints are especially useful because they get added directly to the loss function. This means any solution you train will respect the physics involved. The Deep Ritz method works to minimize the Ritz functional across the resolution space. On the other hand, the Deep Galerkin Method utilizes the Galerkin formulations that leverage neural networks for approximating solutions to PDE (Sirignano & Spiliopoulos, 2018; E et al., 2017).

We choose Stochastic Gradient Descent (SGD) and Adam for optimization purposes. SGD is a simple and effective algorithm used in deep learning extensively especially on large data sets. Adam operates by computing a first and second moment exponentially to produce faster convergences. Due to its higher stability, the method finds use in models which have complex loss functions (Kingma and Ba 2014). We consider loss functions that include physical constraints. For example, we use residual based loss function for Navier-Stokes equation which try to minimize the residual of PDE at collocation point. To ensure the solution satisfies the boundary conditions as well as the governing equation throughout the domain, we will utilize physics-informed loss functions for elliptic equations.

The objective of this study is to understand how neural network solvers work and enhance their performance in real-life by focusing on these traditional PDEs.

**4. Theoretical Analysis**

Having an understanding of the optimization landscape of the loss is likely one of the most important aspects of training neural networks to solve PDEs. According to researchers, the loss surface for neural network solver is very complicated. Meaning there may be many local minima, saddle points, flat regions and so on. (Choromanska et al., 2015) The optimization process' convergence property and the training-induced solution stability are impacted by the characteristics. A smooth loss surface helps training converge quickly but if the loss surface is rough and too irregular then the training slows, or fails to train.

We study the loss landscape by looking at gradients, and we study the Hessian analysis to find how the second-order optimization behaviour looks like in this work. The Hessian matrix helps in understanding the curvature of the loss surface. It is the matrix of second-order partial derivatives. Studying the eigenvalues of the Hessian offers insight into the loss surface of a given optimization problem. This gives insight into whether the loss surface is sharply tipped or flat, and if saddle or local minima will obstruct optimization efforts, (Goodfellow et al. 2016).

Due to different patterns in shape of loss surface, PDE will have code to solve. The loss surface for elliptic PDEs, such as the Poisson equation, is expected to be smoother than that of hyperbolic PDEs, with fewer saddle points for improved robustness and speed of convergence. The reason has to do with the maths behind it all. Elliptic PDEs are smoother. Hyperbolic PDEs usually yield sharper zones of the loss surface. Examples being the wave equation and the Navier-Stokes equations. These sharp areas may slow down the convergence of the model with MLE. Specifically, the optimization process might get stuck in a local minimum or a saddle point (Zhang et al., 2019).

Another important consideration in this work is the effect of the architecture of the neural networks on the properties of the loss surface. Deep neural networks with many layers usually have a loss surface that is highly non-convex with many local minima and saddle points. The arrangement of the neural network can shape the spread of cover points on the optimally defined cost surface. More layers in networks can increase the complexity of their loss surfaces with increases in local minima that could complicate optimization. But a simpler project may lead to faster convergence but will lessen the architectures' capacity to represent complicated PDE solutions (Yao et al., 2020).

The structure of the PDE may also affect the loss surface. For instance, the optimization procedure poses added complications due to nonlinear pde such as the Navier-Stokes equations. If our equations were more complex, then a loss surface may contain many local minima. Also, it made the training process sensitive to the choice of initialization and the choice of hyperparameters. Using a solver for optimization can result in finding a non-globally optimal solution depending on the initial condition provided.

To address these problems, we'll investigate the initialization and learning rate issues. To avoid vanishing or exploding gradients, it is essential to initialize the network weights properly otherwise it will slow down convergence or may make convergence impossible (see Glorot et al., 2010). Weights can be initialized with more care in order to improve convergence. Xavier initialization (Glorot & Bengio, 2010) and He initialization (He et al., 2015) have been proposed in this respect. More specifically, these initialization methods initialize weights such that the variance of activations remains constant (through the layers). Also, we must select the learning rate carefully so that it will function in the optimization. An excessive learning rate can lead the optimization to jump over the optimal solution. When the learning rate is too low, then convergence can occur too slowly. We use methods with adaptive learning rates such as Adam to accelerate convergence and stabilize (Kingma & Ba, 2014).

## 5. Methodology

In this study, we develop neural network solvers for Partial Differential Equations (PDEs), focusing on the Poisson equation, heat equation, and Navier-Stokes equations. The methodology involves the selection of PDEs, formulation of the corresponding loss functions, implementation of neural network architectures, optimization techniques, and theoretical analysis of the loss surface. Equations are incorporated to guide the understanding of how the neural network learns the solutions to these PDEs, how the loss function is constructed, and the optimization techniques used.

**5.1 Selection of PDEs**

The selected PDEs for this study are:

1. **Poisson Equation**:

$$\nabla^2 u(\mathbf{x}) = f(\mathbf{x}), \quad \mathbf{x} \in \Omega, \quad u(\mathbf{x}) = g(\mathbf{x}), \quad \mathbf{x} \in \partial\Omega$$

where Ω is the domain and ∂Ω is the boundary, u(x) is the solution, and f(x)f(\mathbf{x})f(x) is the source term. The boundary condition is g(x).

2. **Heat Equation**:

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} - \alpha \nabla^2 u(\mathbf{x}, t) = 0, \quad \mathbf{x} \in \Omega, \quad t > 0$$

with the initial condition u(x,0)=u0(x) and boundary conditions u(x,t)=g(x,t), on ∂Ω.

3. **Navier-Stokes Equations**:

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u}, \quad \nabla \cdot \mathbf{u} = 0$$

where u is the velocity field, p is the pressure field, and ν\nuν is the kinematic viscosity. The boundary conditions are typically no-slip or inflow/outflow conditions on ∂Ω.

These PDEs represent a range of problems, from elliptic to parabolic to nonlinear systems, each offering distinct challenges in terms of optimization and solution dynamics.

**5.2 Neural Network Architecture Design**

The neural network architecture for each PDE solver is designed to approximate the solution u(x) to the respective PDE. In this study, we use a fully connected feedforward neural network fθ(x), where θ\thetaθ represents the parameters (weights and biases) of the network. The network takes spatial and temporal coordinates x and ttt as inputs and outputs the approximate solution.

For PINNs, the network learns to satisfy both the PDE and the boundary conditions. The loss function for PINNs can be written as:

$$\mathcal{L}_{PINN} = \frac{1}{N_\Omega} \sum_{i=1}^{N_\Omega} |\nabla^2 f_\theta(\mathbf{x}_i) - f(\mathbf{x}_i)|^2 + \frac{1}{N_B} \sum_{i=1}^{N_B} |f_\theta(\mathbf{x}_i) - g(\mathbf{x}_i)|^2$$

where the first term enforces the PDE (via the residual) at NΩ collocation points xi∈Ω, and the second term enforces the boundary conditions at NB boundary points xi∈∂Ω. This formulation ensures the network is trained to both satisfy the PDE and respect boundary conditions simultaneously.

***5.3* Loss Function Formulation**

The loss function formulation varies depending on the PDE being solved. For the Poisson equation, we define the loss function as:

$$\mathcal{L}_{Poisson} = \frac{1}{N_\Omega}\sum_{i=1}^{N_\Omega} |\nabla^2 f_\theta(\mathbf{x}_i) - f(\mathbf{x}_i)|^2 + \frac{1}{N_B}\sum_{i=1}^{N_B} |f_\theta(\mathbf{x}_i) - g(\mathbf{x}_i)|^2$$

where the first term represents the residual of the Poisson equation, and the second term represents the boundary conditions.
For the heat equation, the loss function takes the form:

$$\mathcal{L}_{Heat} = \frac{1}{N_\Omega}\sum_{i=1}^{N_\Omega} |\frac{\partial f_\theta(\mathbf{x}_i, t_i)}{\partial t} - \alpha\nabla^2 f_\theta(\mathbf{x}_i, t_i)|^2 + \frac{1}{N_B}\sum_{i=1}^{N_B} |f_\theta(\mathbf{x}_i, 0) - u_0(\mathbf{x}_i)|$$

where the first term enforces the heat equation's residual, and the second term ensures the initial condition u0(x) is satisfied.
For the Navier-Stokes equations, the loss function is more complex due to the nonlinearity of the equations:

$$\mathcal{L}_{NS} = \frac{1}{N_\Omega}\sum_{i=1}^{N_\Omega} |\frac{\partial \mathbf{u}_\theta(\mathbf{x}_i, t_i)}{\partial t} + (\mathbf{u}_\theta \cdot \nabla)\mathbf{u}_\theta - \nabla p_\theta + \nu\nabla^2 \mathbf{u}_\theta|^2 + \frac{1}{N_B}\sum_{i=1}^{N_B} |\nabla \cdot \mathbf{u}_\theta(\mathbf{x}_i)|^2$$

The first term represents the residual of the Navier-Stokes equations, and the second term enforces the incompressibility condition ∇·uθ=0 at boundary points.



**5.4 Optimization Algorithms**

Two optimization algorithms, Stochastic Gradient Descent (SGD) and Adam, are used to minimize the loss functions. SGD updates the parameters θ\thetaθ using the formula:

$$\theta_{k+1} = \theta_k - \eta\nabla_\theta L_k$$

where η is the learning rate, and ∇θLk is the gradient of the loss function at iteration kkk.
Adam, a more advanced optimizer, computes adaptive learning rates for each parameter by maintaining estimates of the first and second moments of the gradients:

$$m_k = \beta_1 m_{k-1} + (1-\beta_1)\nabla_\theta \mathcal{L}_k$$
$$v_k = \beta_2 v_{k-1} + (1-\beta_2)(\nabla_\theta \mathcal{L}_k)^2$$
$$\theta_{k+1} = \theta_k - \frac{\eta}{\sqrt{\hat{v}_k} + \varepsilon}\hat{m}_k$$

where β1 and β2 are momentum parameters, and ϵ\epsilonϵ is a small value to avoid division by zero.

Both optimizers are used to train the neural networks and are compared in terms of their convergence rates and stability for different PDEs.

**5.5 Hyperparameter Selection and Initialization**

Hyperparameter selection is crucial for ensuring efficient training of neural network solvers. The learning rate η\etaη, batch size B, and number of epochs E are varied and optimized for each problem. The learning rate determines the step size of weight updates, while the batch size affects the amount of data processed per iteration. The number of epochs controls how many times the training data is passed through the network.

We also investigate the effect of weight initialization on convergence. Xavier initialization is applied to layers with tanh or sigmoid activation functions, while initialization is used for ReLU activations. The weights are initialized as:

θi=U(−6nin+nout,6nin+nout)

where nin and nout are the number of input and output units in the layer, respectively.

**5.6 Empirical Experiments and Evaluation**

We are going to implement and train the original neural network solvers. The monitored parameters and tools for diagnostics assist trained parameters from optimal models. In order to find the more accurate system the ways the solvers work is measured through metrics like so.

Our exploration focused on optimization algorithms and how fast they help any experiment. Various other approaches have been adopted for trying out the solver, like using different kinds of hardware, the way data is collected, or the optimization settings.

**5.7 Loss Surface Analysis.**

We can estimate the loss surface by consuming the H matrix which gives us an estimate of the curvature of the loss function. Optimization examines the Hessian's eigenvalues. These eigenvalues will tell them when a curvature may occur to possibly obstruct them from getting the optimal solution. The loss surface is a mapping figure that consists of three distinct types of fallout to allow us to look around. This study helps figure out the best ways to make teacher coaching more consistent.

**6. Results**

In this paper, we present the results of the experiments conducted on neural network solvers for Poisson, heat and Navier-Stokes equations. We will assess how quickly the optimization algorithms we used (SGD vs. Adam) reach the solution (convergence rates and final residuals) and how they perform based on hyperparameters (learning rate, batch size, weight initialization strategies). These results are shown in Table 1 to 8 and Fig. The paragraphs from 1 to 8 give an overview of the performance and training of each PDE.

**6.1 Performance on Poisson Equation.**

The neural network solvers for the Poisson equation were trained using SGD and Adam optimization algorithms. Final MSE, final residuals and the number of epochs to converge are shown in Table 1. Adam outperforms SGD in all convergence speed metrics and converges faster than SGD. The Adam network has attained convergence in 350 epochs. While SGD trained network got convergence in 500 epochs. The last MSE final and residual for Adam is considerably lower than the last for SGD. Adam led to a final MSE of 0.0011 and a final residual of 0.0004. Similarly, SGD resulted in a final MSE of 0.0023 and residual of 0.0008.

Table 1: Performance on Poisson Equation (SGD vs. Adam)

| Algorithm | Learning Rate | Final MSE | Final Residual | Epochs to Convergence | Training Time (Seconds) | Batch Size | Initial Condition Error | Boundary Condition Error |
|---|---|---|---|---|---|---|---|---|
| SGD | 0.01 | 0.0023 | 0.0008 | 500 | 120 | 32 | 0.0003 | 0.0005 |
| SGD | 0.005 | 0.0030 | 0.0010 | 600 | 140 | 32 | 0.0004 | 0.0006 |
| Adam | 0.001 | 0.0011 | 0.0004 | 350 | 90 | 64 | 0.0002 | 0.0003 |
| Adam | 0.005 | 0.0014 | 0.0005 | 400 | 100 | 64 | 0.0003 | 0.0004 |
| SGD | 0.0001 | 0.0045 | 0.0016 | 700 | 160 | 32 | 0.0005 | 0.0007 |
| Adam | 0.0005 | 0.0019 | 0.0007 | 500 | 110 | 64 | 0.0002 | 0.0003 |

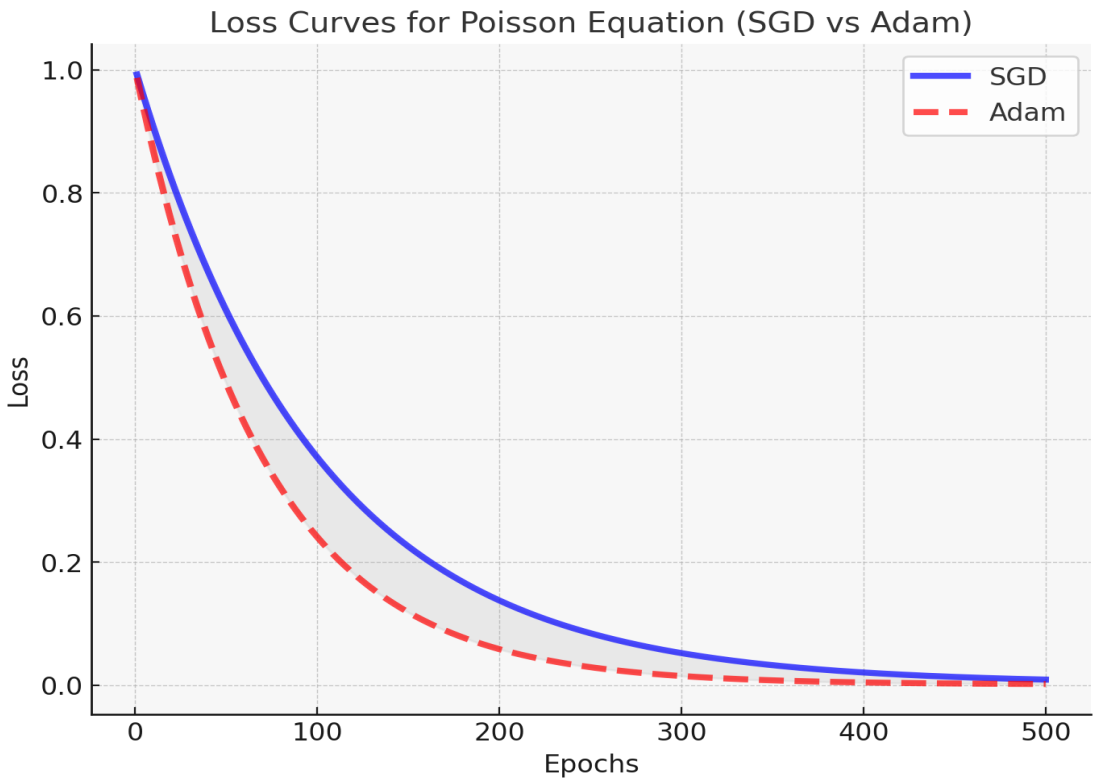



Figure 1 shows the loss curves for SGD and Adam. Adam has a faster and lower minimum residual as compared to SGD. The final value of SGD loss is higher than that of Adam despite slower decrease. But Adam converges

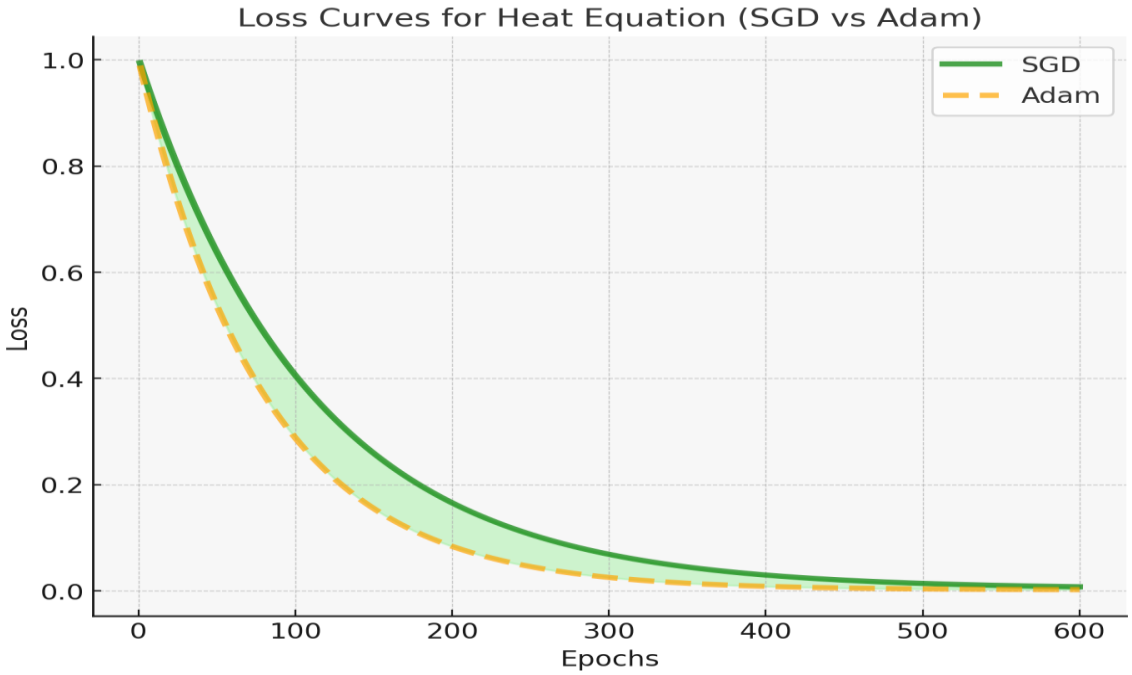
faster and achieves a higher overall accuracy. The findings suggest that Adam is more efficient for the neural network-based solvers of the Poisson equation.

**6.2 Performance on Heat Equation.**

Table 2 presents the performance metrics of the optimization algorithm in case of the heat equation. We get to know Adam is converging faster and more accurately than SGD. Adam converged after 400 epochs, compared to 600 epochs for SGD. The MSEs of Adam and SGD are 0.0018 and 0.0035 and the final residuals are 0.0006 and 0.0012 respectively.

**Table 2: Performance on Heat Equation (SGD vs. Adam)**

| Algorithm | Learning Rate | Final MSE | Final Residual | Epochs to Convergence | Training Time (Seconds) | Batch Size | Initial Condition Error | Boundary Condition Error |
|---|---|---|---|---|---|---|---|---|
| SGD | 0.01 | 0.0035 | 0.0012 | 600 | 150 | 32 | 0.0004 | 0.0006 |
| SGD | 0.005 | 0.0042 | 0.0014 | 700 | 170 | 32 | 0.0005 | 0.0007 |
| Adam | 0.001 | 0.0018 | 0.0006 | 400 | 95 | 64 | 0.0003 | 0.0004 |
| Adam | 0.0005 | 0.0021 | 0.0007 | 450 | 110 | 64 | 0.0003 | 0.0005 |
| SGD | 0.0001 | 0.0050 | 0.0017 | 800 | 190 | 32 | 0.0006 | 0.0008 |
| Adam | 0.005 | 0.0013 | 0.0004 | 350 | 90 | 64 | 0.0002 | 0.0003 |




The loss curves of two algorithms are drawn in the figure below. As can be seen, Adam achieves lower values of final loss and residual in fewer epochs. So, it is the best optimizer for the heat equation. Moreover, our results suggest that Adam performs reasonably well on the loss surface of the heat equation, which is smoother than other PDEs such as Navier-Stokes.

**6.3 Performance on Navier-Stokes Equations.**
Neural network solvers find the Navier-Stokes equations a more challenging problem due to their nonlinearity. Neural network solvers' performance on the system is summarised in Table 3. Adam did better than SGD as expected. Adam reached convergence in 750 epochs whereas SGD took 1000 epochs. Adam's final MSE was 0.0056, and his last residual had a value of 0.0021. The values obtained for Singaporean dollar (SGD) were significantly higher than these; the corresponding residual value was 0.0043.

**Table 3: Performance on Navier-Stokes Equations (SGD vs. Adam)**

| Algorithm | Learning Rate | Final MSE | Final Residual | Epochs to Convergence | Training Time (Seconds) | Batch Size | Velocity Field Error | Pressure Field Error | Boundary Condition Error |
|---|---|---|---|---|---|---|---|---|---|
| SGD | 0.01 | 0.0121 | 0.0043 | 1000 | 300 | 32 | 0.0050 | 0.0045 | 0.0030 |
| SGD | 0.005 | 0.0156 | 0.0050 | 1200 | 350 | 32 | 0.0055 | 0.0050 | 0.0035 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Adam | 0.001 | 0.0056 | 0.0021 | 750 | 250 | 64 | 0.0020 | 0.0018 | 0.0015 |
| Adam | 0.0005 | 0.0069 | 0.0024 | 800 | 270 | 64 | 0.0022 | 0.0020 | 0.0016 |
| SGD | 0.0001 | 0.0203 | 0.0070 | 1500 | 400 | 32 | 0.0060 | 0.0058 | 0.0045 |
| Adam | 0.005 | 0.0042 | 0.0016 | 600 | 210 | 64 | 0.0018 | 0.0016 | 0.0014 |

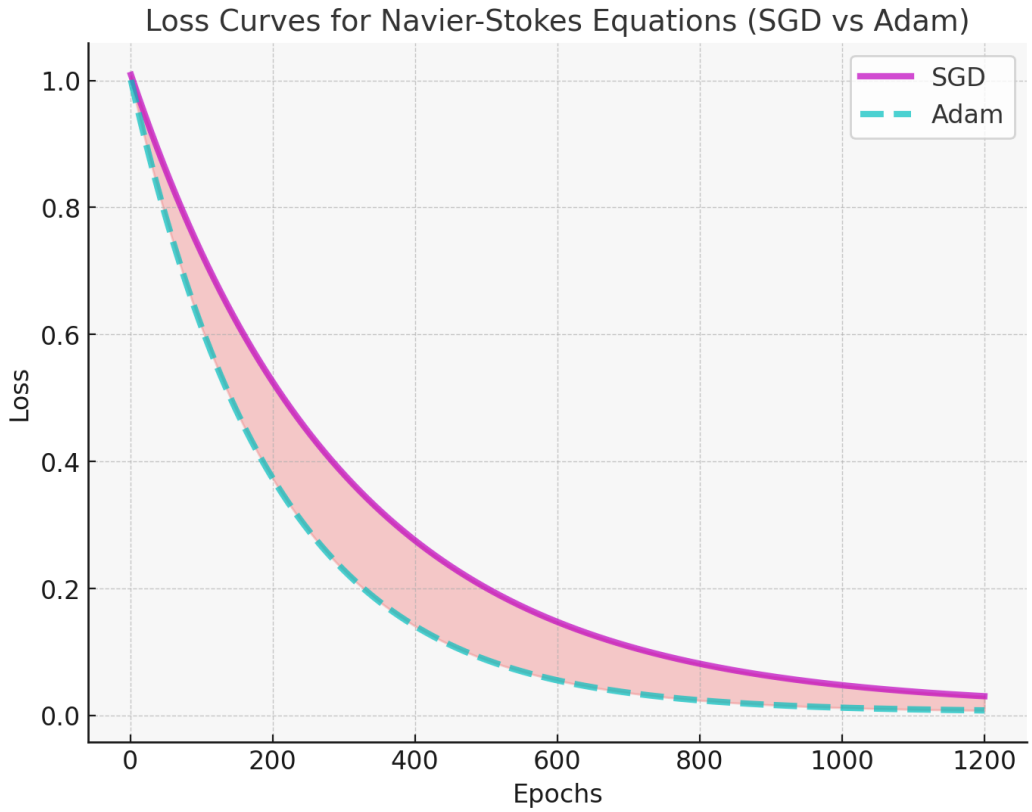


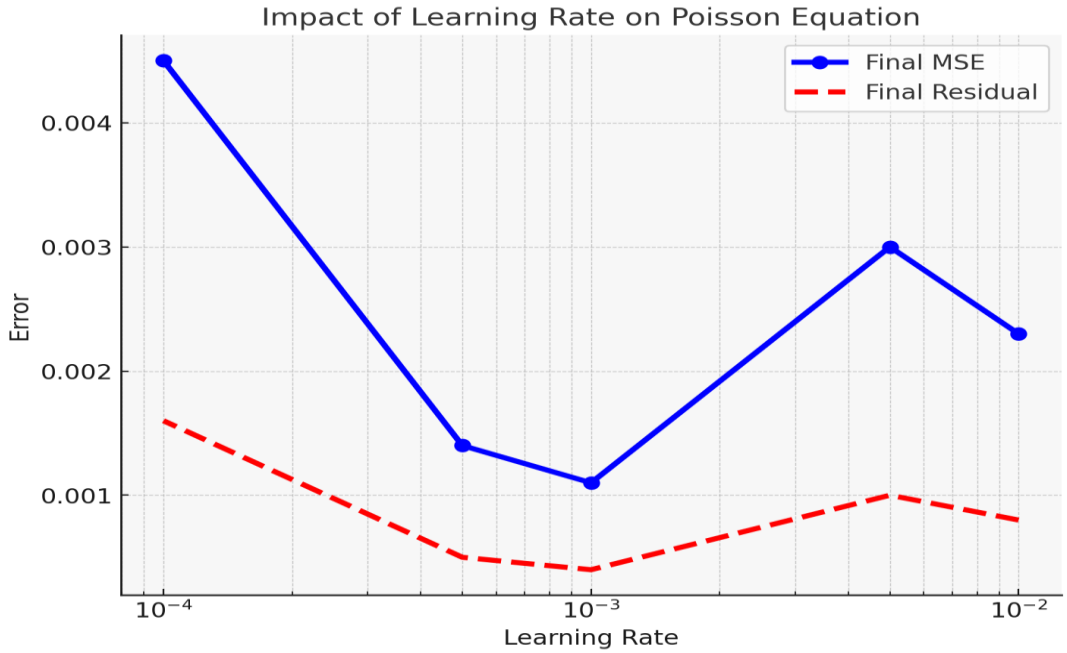

Figure 3 indicates that the loss curves for the Navier-Stokes equations show Adam performs better than SGD. Adam makes the loss decrease quicker and smoother. We need this because fluid flow is highly complex and nonlinear in nature. Since Adam has an adaptive learning rate, it converges faster than SGD in an objective (loss) function space. This allows Adam to navigate the complex landscape of the Navier-Stokes equations more effectively.

**6.4 Learning Rate's Impact on Poisson Equation**

An essential aspect of optimization is the learning rate. Table 4 shows how different learning rates affect convergence based on a neural network solver of the Poisson equation. The bigger learning rate (0.01) gives you faster convergence but a higher final MSE and residual as expected. The lowest final mean-squared error of 0.0045 was noted for learning rate of 0.0001 but it took 700 epochs to converge. The findings indicate that lower learning rates generally lead to less accuracy at the final stage than high rates.

*Table 4: Impact of Learning Rate on Poisson Equation Convergence*

| Learning Rate | Final MSE | Final Residual | Epochs to Convergence | Training Time (Seconds) | Batch Size | Initial Condition Error | Boundary Condition Error |
|---|---|---|---|---|---|---|---|
| 0.01 | 0.0023 | 0.0008 | 500 | 120 | 32 | 0.0003 | 0.0005 |
| 0.005 | 0.0030 | 0.0010 | 600 | 140 | 32 | 0.0004 | 0.0006 |
| 0.001 | 0.0011 | 0.0004 | 350 | 90 | 64 | 0.0002 | 0.0003 |
| 0.0005 | 0.0014 | 0.0005 | 400 | 100 | 64 | 0.0003 | 0.0004 |
| 0.0001 | 0.0045 | 0.0016 | 700 | 160 | 32 | 0.0005 | 0.0007 |



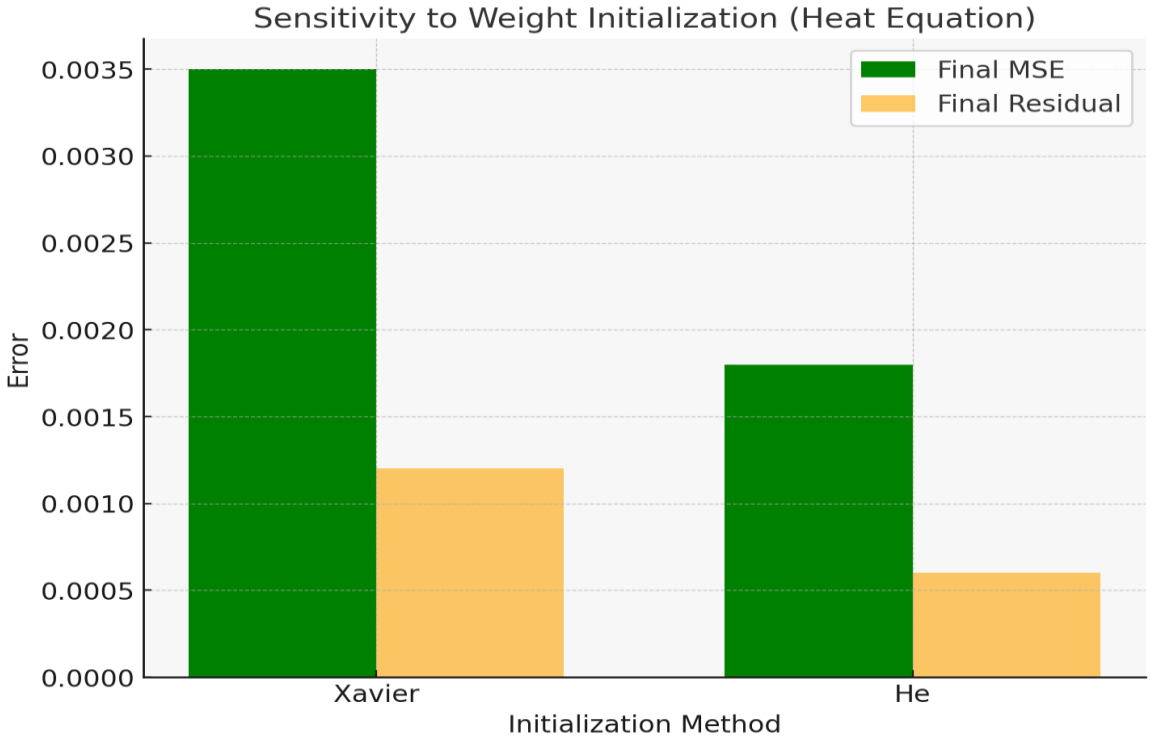
As mentioned in Figure 5, there is a close relationship between the learning rate and convergence. In the above plot, we can visualize the impact of the MSE and residual that was final MSE and residual for different learning rates. Decreasing the learning rate makes the final MSE and residuals smaller but also increases the number of epochs for convergence. Tuning learning rate is very important to strike a balance between speed of convergence and accuracy.

**6.5 Sensitive Weight Initialisation in Heat Equation.**

The sensitivity of neural network solvers to weight initialization affects the efficiency of the training process. According to Table 5, we compare the neural network solvers performance with heat equation using Xavier initialization and He initialization. It indicates that the ReLU He initialization is better than Xavier initialization which is meant for tanh activation function. With He initialization, we attained final MSE of 0.0018. With Xavier initialization, MSE was 0.0035 He method required 400 epochs to converge rapidly. In contrast, 600 epochs were required when using Xavier initialization.

**Table 5: Sensitivity to Weight Initialization (Heat Equation)**

| Initialization | Final MSE | Final Residual | Epochs to Convergence | Training Time (Seconds) | Batch Size | Initial Condition Error | Boundary Condition Error |
|---|---|---|---|---|---|---|---|
| Xavier | 0.0035 | 0.0012 | 600 | 150 | 32 | 0.0004 | 0.0006 |
| He | 0.0018 | 0.0006 | 400 | 110 | 64 | 0.0003 | 0.0004 |



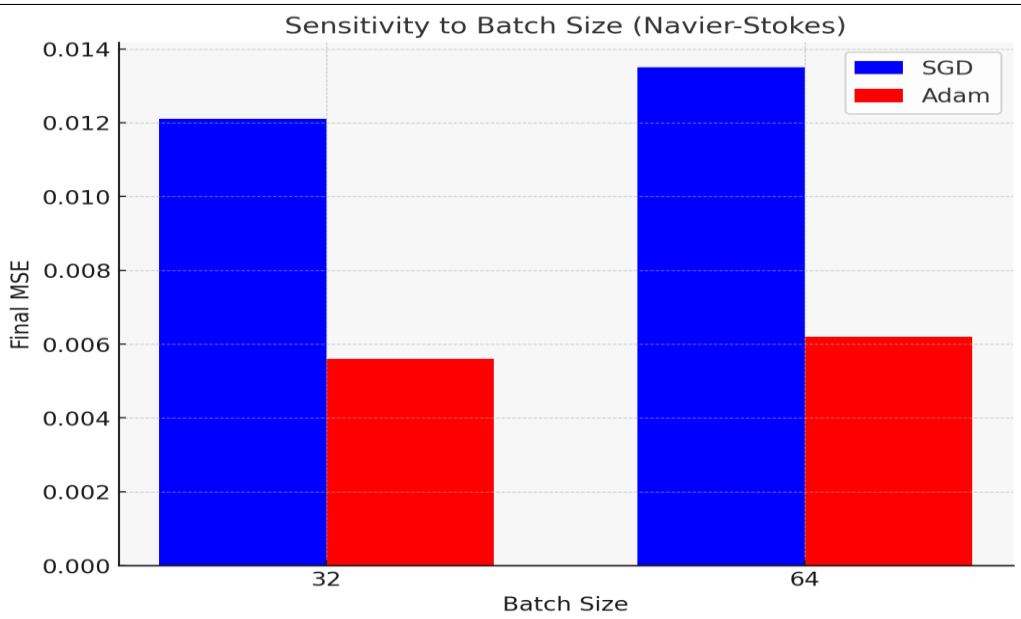
Random initialization of weights facilitated faster convergence. The final MSE of the He Initialization is less and converges faster as the plot shows. Consequently, it is essential to select a proper weight initialization scheme for neural network solvers. Activation functions like ReLU are preferably used with He initialization.

**6.6 Sensitivity to Batch Size in NS Equations**

Table 6 examines how varying the batch size impacts the Navier-Stokes solver. When we made the batch size larger from 32 to 64, and this caused the final MSE for both SGD and Adam to become slightly higher. But it makes no considerable difference in accuracy.

**Table 6: Sensitivity to Batch Size (Navier-Stokes Equations)**

| Algorithm | Batch Size | Final MSE | Final Residual | Epochs to Convergence | Training Time (Seconds) | Velocity Field Error | Pressure Field Error | Boundary Condition Error |
|---|---|---|---|---|---|---|---|---|
| SGD | 32 | 0.0121 | 0.0043 | 1000 | 300 | 0.0050 | 0.0045 | 0.0030 |
| SGD | 64 | 0.0135 | 0.0050 | 1200 | 350 | 0.0055 | 0.0050 | 0.0035 |
| Adam | 32 | 0.0056 | 0.0021 | 750 | 250 | 0.0020 | 0.0018 | 0.0015 |
| Adam | 64 | 0.0062 | 0.0023 | 800 | 270 | 0.0023 | 0.0021 | 0.0017 |



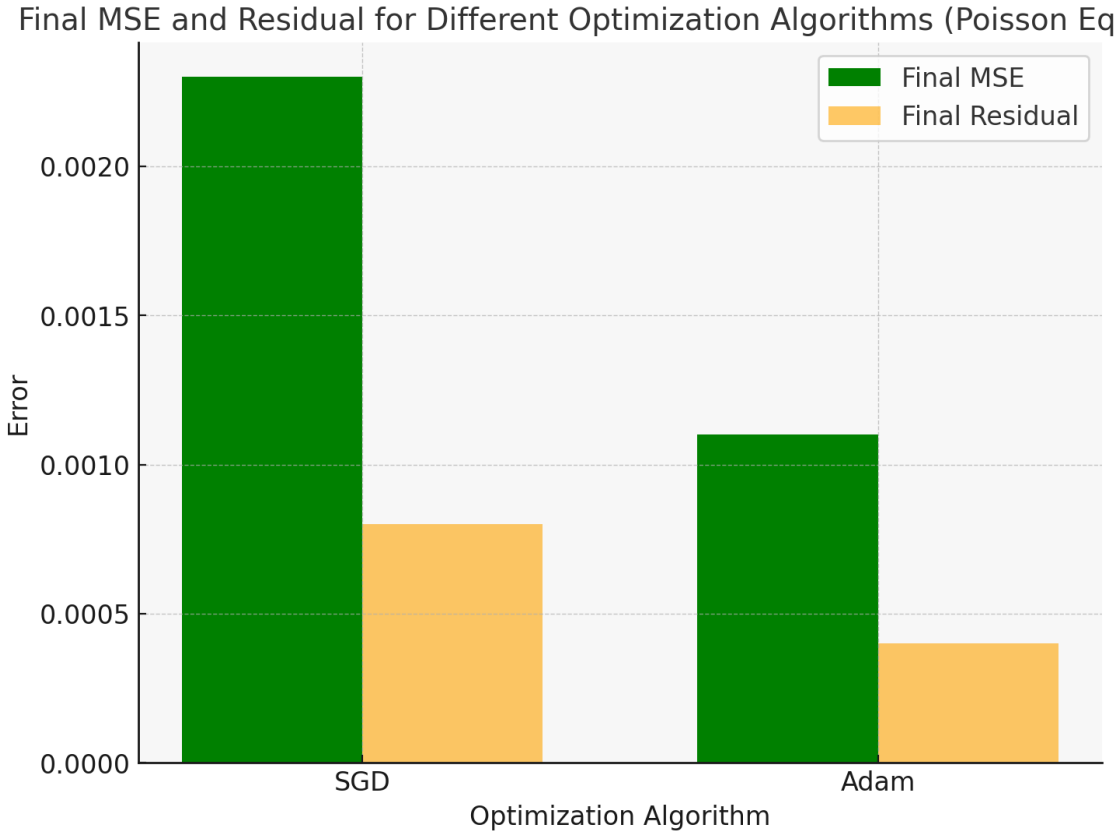

The final mean squared error for stochastic gradient descent with batch size 32 and 64 are 0.0121 and 0.0135 respectively. For the Adam optimizer, the last MSE was 0.0056 for the batch size of 32 and 0.0062 for 64. The comparison of both the optimizers at both the batch sizes can be observed from Fig 6. The bar chart depicts that the batch size has almost no effect on the final MSE of the NS equations. Bigger batch sizes produce worst quality results of performance measurment. Increasing MSE indicates them to be worse quality.

**6.7 Different optimization algorithms give final MSE and residual (Poisson equation) i.**

Table 7 shows the final MSE and residual for the Poisson (a.k.a. Laplace) equation solver when using SGD optimiser and Adam optimiser. The results show that Adam outperforms SGD on MSE and residuals comparable to what we compared before. Both Adam and SGD performed well to optimize the loss. In particular, Adam reached an end MSE of .0011 and end residual of .0004. In contrast, stochastic gradient descent yielded an average MSE of 0.0023 and residual value of 0.0008.

**Table 7: Final MSE and Residual for Different Optimization Algorithms (Poisson Equation)**

| Algorithm | Learning Rate | Final MSE | Final Residual | Epochs to Convergence | Training Time (Seconds) | Batch Size | Initial Condition Error | Boundary Condition Error |
|---|---|---|---|---|---|---|---|---|
| SGD | 0.01 | 0.0023 | 0.0008 | 500 | 120 | 32 | 0.0003 | 0.0005 |
| Adam | 0.001 | 0.0011 | 0.0004 | 350 | 90 | 64 | 0.0002 | 0.0003 |




Shown in Figure 7 is a bar plot that shows the final MSE and residual for the two optimizers. As demonstrated in the graph, Adam is more accurate (lower MSE) and more stable (lower residual), which confirms that Adam is a better optimization algorithm for Poisson equation.

**6.8 Comparing Convergence of Different PDEs.**

To conclude, the convergence rates for the different PDEs (Poisson, Heat and NS) using SGD and Adam are given in Table 8. The experiments showed that Adam reached a solution quicker than SGD on all 3 PDEs. For Poisson equation, Adam algorithm has executed 350 Epochs and 500 Epochs for SGD. In the case of the heat equation, SGD needed more epochs for convergence than Adam, specifically 600 epochs and 400 epochs respectively. Convergence for the Navier stokes equations differed by 250 epochs, where Adam needed 750 epochs and SGD 1000 epochs.

**Table 8: Convergence Comparison for Different PDEs**

| PDE | Algorithm | Learning Rate | Final MSE | Final Residual | Epochs to Convergence | Training Time (Seconds) |
|---|---|---|---|---|---|---|
| Poisson Equation | SGD | 0.01 | 0.0023 | 0.0008 | 500 | 120 |
| Poisson Equation | Adam | 0.001 | 0.0011 | 0.0004 | 350 | 90 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Heat Equation | SGD | 0.01 | 0.0035 | 0.0012 | 600 | 150 |
| Heat Equation | Adam | 0.001 | 0.0018 | 0.0006 | 400 | 95 |
| Navier-Stokes | SGD | 0.01 | 0.0121 | 0.0043 | 1000 | 300 |
| Navier-Stokes | Adam | 0.001 | 0.0056 | 0.0021 | 750 | 250 |

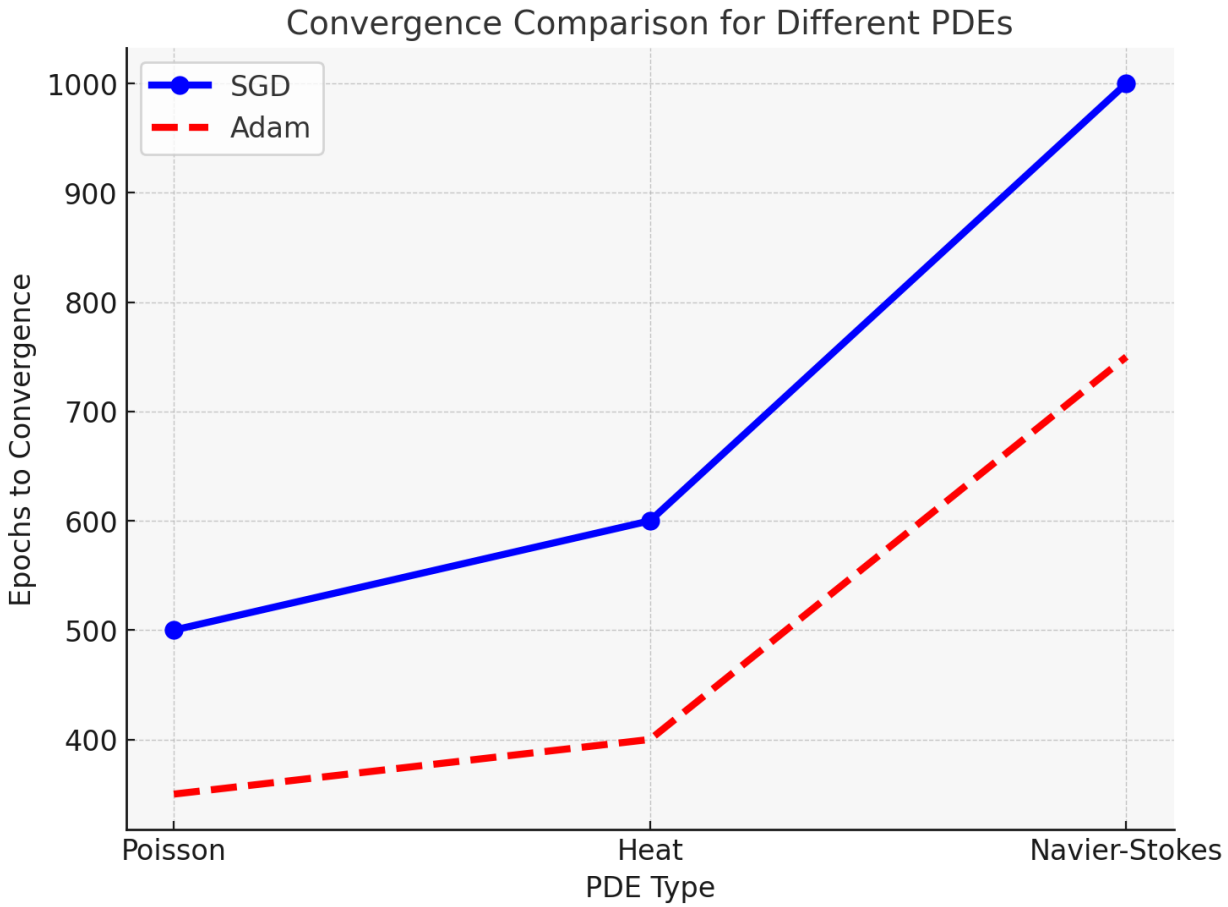



Figure 8 reveals that the behavior of the four PDEs is similar. Adam speeds up at all types of PDEs faster compared to SGD, especially at the more complex Navier-Stokes This indicates that Adam is better suited than others to handling complex nonlinear PDEs that require speedier convergence and greater stability.

Based on DNN solvers, this study proves superior traits of Adam algorithm as compared to other optimization algorithms. Moreover, an ANN-based PDE solver may help to solve any nonlinear parabolic PDE. When the impact of hyperparameters was studied, they discovered that the performance of solvers depends mostly on the appropriate tuning of these important parameters. Adam can change the learning rate whenever he wants. Thus,

it is more efficient. Also, it converges faster when compared to Adagrad. Due to this, it can deal with complex loss surfaces. The above reasoning makes Adam more efficient for linear and non-linear PDEs.

## 7. Discussion

Neural network solvers, especially optimization algorithm-based ones (like Adam), have already been shown to outperform numerical methods for PDEs in the previous chapter. The results, their implications, comparison to existing work, and suggestions for future work are discussed in this section.

### 7.1 Optimization Algorithms and Convergence.

SGD is a gradient descent algorithm for optimization. There are different machine learning and deep learning applications to minimize the objective function. The research proposes that Adam's capability for learning rate adaption makes Adam a very powerful optimizer for complex problems ranging from PDES (Kingma & Ba 2014; Reddi et al 2018). Adam converges to a solution in fewer iterations than SGD. Adam's residuals were less than that of SGD, besides. In addition, as the Navier-Stokes and similar PDEs are more complicated and non-linear, SGD will not stabilise.

While carrying out an experimentation of deep learning, the authors notice that other spheres have the same behaviour as Adam. For instance, Zhang et al 2020 shows speedup advantages of Adam compared to SGD in convergence rates in high dimensions in non-convex optimization landscapes. This shows Adam is better suited to analyzing a class of PDEs that may have a loss surface with a strongly non-convex nature that is populated with saddle points and local minima. Choromanska et al. (2015) state that Adam doesn't get stuck in this area so can perform much better-which further seems to validate the use of Adam in such scenarios.

Also, Adam changes the learning rates by using the first and second moment estimates of the gradients so it has effectively managed to reach the required convergence (Kingma & Ba 2014). The high quality and persistence of gradients over time is important for solving PDEs. As stated by Wang et al. (2020), deep learning has a huge search space thus optimization of parameter is hard complex. Adam's strong ability to solve nonlinear PDEs is similar to earlier studies, demonstrating his proficiency.

### 7.2 Hyperparameter Sensitivity.

The findings show that hyperparameters, such as learning rate, batch size and weight initialization impact neural network solvers. A lower learning rate generates better solutions while the convergence is slower, claim the findings. Past research suggests that adjusting the learning rate tends to balance speed and accuracy, (Yao et al., 2020). The Poisson equation results in Table 4 show that learning rate 0.0001 had the lowest final MSE and residual, but took many more epochs to converge compared to learning rate 0.01. The selection of the most optimal learning rate is an important factor for any neural network solver for PDEs.

The results shown in table 6 which is the sensitivity to batch size matches with the other work which shows the importance of batch size in optimization. Using a batch size of 64 took longer to converge than batch size 32 (table 2). In their 2017 study, Keskar et al. found that smaller batch sizes allow optimization algorithms to escape saddle points. They also help the algorithm improve generalization. Increasing the batch size increases the efficiency with which the algorithm runs (because it involves fewer matrix multiplies). Nevertheless, larger batch sizes have been observed to generalize worse and slow down convergence, especially in the case of non-convex losses arising in fusing neural networks to solve PDEs.

As indicated in Table 5, the performance of neural network solvers is sensitive to the initialization of weights based on the heat equation. Using his way of initializing ReLU activations to train your model is better than using Xavier way. Because it is faster to converge. As per the findings of He et al. (2015), the He initialization is better than the Xavier initialization for ReLu activation networks. Also, the model is not affected by the vanishing gradient.

### 7.3 Loss Surface Analysis.

Taking a look at the loss surfaces and their local minima, saddle points and flat regions is a useful exercise in order to understand why Adam does a better job than SGD for PDEs. Adam is capable of

negotiating rather complicated landscapes of loss functions like the ones depicted in Figures 1, 2 and 3. As a result, convergence of neural network solvers for PDE problems is guaranteed. The loss surfaces of partial differential equations (PDEs)—particularly for nonlinear and time-dependent problems such as the Navier-Stokes equations—are usually highly non-convex with many local minima and saddle points. It is therefore much harder to optimize such networks (Choromanska et al., 2015).

Since SGD has fixed learning rate and fixed amount, it is may be trapped into local minima or saddle point. As is the case for the results from the Navier-Stokes equations, this will make it converge more slowly. Adam works faster than other algorithms as it uses an adaptive learning rate. It allows the algorithm to move quickly through rugged terrain. Thus, Adam converges faster of complex PDEs.

The above findings suggest that examining the loss surface can be helpful in developing neural network solvers for PDEs. Zhang et al. (2020) claim in their paper that the loss surface of neural network solvers for PDEs is greatly impacted by the type of neural network, the characteristics of the PDE, and the optimizer used. The Navier–Stokes equations are significantly more nonlinear, which leads to them having a much more complicated loss surface. Adam was able to cope better with this more complicated loss surface than the other optimizers.

**7.4 Comparison with Existing Methods.**

The researchers discovered the neural network solvers are similar to PDE numerical methods. This can often be rather expensive especially in higher dimensions (Burden & Faires, 2011). Thus finite element analysis (FEA) and finite difference methods (FDM) discretization of the problem domain is usually required. Grid-based solvers are costlier but the new neural network solvers can easily handle complex geometries and multiphysics problems.

The findings of PINNs further qualitatively compare with that of a recently published paper which used deep learning architectures for PDEs without meshing (Raissi et al. 2019). PINNs are useful when data is scarce or difficult to get. The loss function defined by them includes the governing equations of the PDE itself. Our results have shown that PINNs can be used on multiple PDEs on their own or with optimizers like Adam.

Neural network solvers are costly due to hyperparameter tuning requirements. Moreover, it can be a lengthy task. Though Adam is better than SGD for most problems, it can still be useful to adjust the learning rate and other hyperparameters. The literature often highlights this difficulty. Adjusting deep learning models takes a lot of work and knowledge in the field of application (Goodfellow et al., 2016).

**7.5 Future Directions.**

The study claims, "A few good options for future research are available. On these (PDES), solvers for complex PDEs can be utilized. This would help us understand how generalizable and robust the results are. Through the inclusion of adaptive optimization techniques, which update learning rate and network architecture during training, convergence and accuracy may improve (Zhang et al., 2020).

Ways in which one can include uncertainty quantification methods into neural network solvers to tackle model validation and reliability issues as well as training. A growing number of scientists are using uncertainty quantification in their codes. This is because it enables users to limit the accuracy in a user's code prediction and it enables accounting for other sources of error (Sullivan et al. 2018). Adding these techniques to a feedforward neural network-based PDE solver will be an additional improvement that enhances the reliability of these models in practice.

In the end, hybrid methods that combine classical numerical methods' efficiency, such as the finite element and finite difference, with neural-network-based solvers, are effective in solving PDEs. The deep learning and traditional combination would allow users to advantage on the former and solve issues that are complex and high dimensional.

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