Project 3 - Report

Course: Hochleistungsrechnen für Maschinelles Lernen

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This technical report contains the names of our group members as well as a performance comparison between the single global PINN from project 1 and the GatedPINN approach in this project. Generated figures will not be incorporated in the project pdf so as to fit the page length requirement and can be found as cell outputs in the notebook file or as saved figures in the repository.

1. Introduction

This project investigates how Physics-Informed Neural Networks (PINNs) can be used to solve differential equations. Specifically, it focuses on the extension of PINNs through a gate network to enable the modeling of partial solutions in subdomains. The objective is to implement, train, and evaluate a GatedPINN for the one-dimensional heat equation and compare its performance to that of the single global PINN from project 1.

2. Problem Statement

The underlying physical problem is the one-dimensional heat equation:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

with the analytical solution:

$$u(x,t) = \sin(\pi x) e^{-\pi^2 t}$$

The initial condition is: $u(x,0) = \sin(\pi x)$

The boundary conditions are: $u(0,t) = u(1,t) = 0$

The goal is to approximate this equation using neural networks and evaluate the prediction quality using different methods.

3. Methodology

3.1 Physics-Informed Neural Networks (PINNs)

The base model consists of a feedforward neural network with three hidden layers, each with 100 neurons and "tanh" activation functions. The PINNs are trained using a loss function that incorporates the PDE residual as well as the initial and boundary conditions.

3.2 Domain Decomposition

The solution domain is split into two subdomains: $\Omega_1 = [0, 0.6]$ and $\Omega_2[0.4, 1]$ with an overlapping region of $[0.4, 0.6]$. Each subdomain is handled by a separate PINN expert.

3.3 Gated PINN

A gate network with two hidden layers of 20 neurons each is used. The gate network determines the weighting of the two experts at each point through a softmax layer. The combined prediction results from a weighted sum of the experts' outputs.

4. Results

4.1 Expert Training

The experts were trained for 1000 epochs each. By incorporating additional initial and boundary condition losses, the experts achieved qualitatively reasonable approximations of the solution.

4.2 Gated PINN Prediction

The Gated PINN predictions were compared to the exact solution across multiple time slices (every 0.1 seconds). The plots show good agreement between the GatedPINN predictions and the analytical solution.

4.3 Gate Behavior

The visualization of the gate weights shows a meaningful distribution. Expert 1 dominates in the region $x < 0.4$, while Expert 2 dominates in $x > 0.6$. A smooth transition between experts occurs in the overlapping region.

5. Discussion

The results demonstrate that GatedPINN is capable of reliably approximating the solution to the heat equation. The use of the gate network is particularly advantageous, enabling a smooth transition between experts.

When comparing the output of the GatedPINN with that of the single global PINN from project 1, it can easily be seen that the GatedPINN performs noticeably better. The prediction better represents the numerical solution, especially when looking at the boundaries i.e. $x = 0$ and $x = 1$.

While the GatedPINN approach produces the better prediction, it has to be noted that the training took more of an effort when compared to the single PINN. Challenges included stabilizing the training of the PINN experts and achieving a meaningful distribution of gate weights. Potential improvements could involve a deeper investigation into the influence of subdomain partitioning and gate network architecture.

6. Conclusion

GatedPINN proved to be an effective method for solving the one-dimensional heat equation. By combining subdomain specialization and gate weighting, the model achieved high predictive accuracy, better than that of the single global PINN. This approach is especially suitable for problems with clearly separable partial solutions and provides a solid foundation for applications to more complex PDEs.