Topological Neuroevolution of Physics-informed Neural Networks

Introduction

- Neural networks can be biased towards various solutions in several ways.
- One such way to bias neural networks is through their structure (e.g., as in convolutional neural networks).
- In this project, I evolved the structure of physics-informed neural networks (PINNs) using the NeuroEvolution of Augmenting Topologies (NEAT) algorithm to add such a structural bias.

Background

- PINNs are neural networks that can integrate noisy data with prior physics knowledge, and NEAT is an algorithm for evolving the node-by-node graph structure (i.e., topology) of a neural network.

PHYSICS-INFORMED NEURAL NETWORKS

- For a partial differential equation (PDE) of the form $\mathcal{N}[u;\ \theta] = g$ (where $\mathcal{N}$ is a nonlinear differential operator and u is the solution of the PDE), a PINN contains, in essence, two networks: an ordinary feed-forward network that approximates $u(t,\ x)$, and a residual network that encodes the residuals of the PDE ($R = \mathcal{N}[u,\ \theta] - g$).
- For any solution that respects a PDE, the residuals of that PDE are 0, so when the residuals are minimized, the solution respects the PDE, and thus the physics described by the PDE.
- The loss used to train the PINN is the MSE loss of both networks combined.

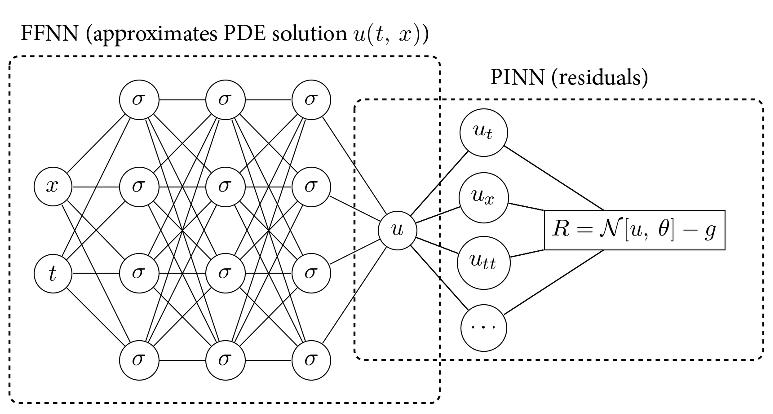

Figure 1: PINN architecture. Diagram created by author.

Specifically, the loss is $L = \text{MSE}_u + \text{MSE}_r$, where MSE_u is a typical mean-squared error from the available data (generally used to enforce initial and boundary conditions), and MSE_r is the mean-squared error of the residuals of the PDE governing the system, evaluated at a finite distribution of collocation points.

$\text{MSE}_f = \frac{1}{N_u} \sum_{i=1}^{N_u} \left\| f(t_f^i,\ x_f^i) \right\|^2$, where $f(t_f^i,\ x_f^i) = R = \mathcal{N}[u,\ \theta] - g$, and $t_f^i,\ x_f^i$ are the collocation points.

$\text{MSE}_u = \frac{1}{N_u} \sum_{i=1}^{N_u} \left\| u(t_u^i,\ x_u^i) - u^i \right\|^2$, where $\{t_u^i,\ x_u^i,\ u_i\}$ are the available data.

NEUROEVOLUTION OF AUGEMENTING TOPOLOGIES

- The Neuroevolution of Augmenting Topologies (NEAT) algorithm is a genetic algorithm that evolves neural network topologies and weights simultaneously.
- NEAT starts with an "empty" network (fully connected between input and output with no hidden nodes), and then iteratively adds individual neurons and connections.
- NEAT tracks the history of genes to enable crossover between homologous structures.
- NEAT utilizes speciation to prevent new topologies from being immediately discarded. Adding a new neuron to a network will cause the fitness to decrease because the weights of the network have not yet adjusted to the new structure. To solve this, NEAT separates significantly different network topologies into different species with internal competition.
- In the context of this project, the fitness is the negative PINN loss.

Engineering Goals

- The first goal of this project is to accurately approximate a variety of physics systems using NEAT-evolved PINNs.
- The second goal of this project is to use a system involving NEAT-evolved PINNs to achieve state-of-the-art performance approximating systems involving high frequency functions.

Methods

- The python-neat package (for the NEAT algorithm) and the jax package (for auto-differentiation) were used.
- A custom (jax-compatible) evaluation function for the irregular neural networks was built and then differentiated and used.
- The neural networks were evaluated against a reference solution for each equation, and L2 errors were calculated.

Results

[attached on poster to be removeable; see figures]

Discussion

- Overall, the NEAT-evolved PINNs successfully approximated the physics systems.
- On average, they had lower accuracy than traditional methods but used fewer parameters.

Conclusion

- NEAT-evolved PINNs can be used in applications that require parameter-efficient simulation (i.e., where very low computational cost is necessary) of physical systems governed by differential equations.
- Future research should explore ways to increase the performance and improve convergence of NEAT-evolved PINNs.