Scientific Machine Learning for the No-Three-In-Line Problem

Pranav SciML Project Roadmap

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1 Overview

The No-Three-In-Line problem is a classical combinatorial optimization challenge that involves placing as many points as possible on an $n \times n$ grid such that no three points lie on a straight line. This project aims to reformulate the problem using Scientific Machine Learning (SciML) by modeling point placement and learning dynamics through differential equations and energy-based methods.

2 Formulation

We represent the relaxed decision of placing a point at grid location (i, j) with a continuous variable $x_{ij}(t) \in [0, 1]$, and introduce an energy-based differential system to evolve these variables over time while discouraging invalid collinear placements.

Energy Function

$$E(x(t)) = \sum_{(i_1,j_1),(i_2,j_2),(i_3,j_3)\in\mathcal{L}} \alpha \cdot x_{i_1j_1}(t) \cdot x_{i_2j_2}(t) \cdot x_{i_3j_3}(t) \tag{1}$$

Where:

- $\mathcal{L}$: Set of all triplets of collinear points on the grid.
- α: Penalty coefficient ($\alpha > 0$).

Dynamics

$$\frac{dx_{ij}}{dt} = -\frac{\partial E}{\partial x_{ij}} + \eta(t) \tag{2}$$

$\eta(t)$ represents exploratory noise (e.g., Gaussian).

3 Classical Optimization

To link with classical optimization, we consider:

$$\max \sum_{i,j} x_{ij} \tag{3}$$

Subject to:

$$x_{i_1 j_1} + x_{i_2 j_2} + x_{i_3 j_3} \leq 2 \quad \forall (i_1, j_1), (i_2, j_2), (i_3, j_3) \in \mathcal{L} \tag{4}$$

4 Learning Model

Let $\theta(t)$ be the internal representation or parameters used by PatternBoost. We define a learning loss $\mathcal{L}(\theta; x(t))$ that penalizes invalid patterns and suboptimal placements.

Learning Rule

$$\frac{d\theta}{dt} = -\nabla_\theta \mathcal{L}(\theta; x(t)) + \zeta(t) \tag{5}$$

$\zeta(t)$ represents stochastic perturbation for learning exploration.

5 Combined System

A joint SciML formulation combining grid placement and learning:

$$\frac{dx_{ij}}{dt} = -\frac{\partial E}{\partial x_{ij}} + \eta(t) \tag{6}$$

$$\frac{d\theta}{dt} = -\nabla_\theta \mathcal{L}(\theta; x(t)) + \zeta(t) \tag{7}$$

6 Objectives

1. Develop and solve the differential equation-based model for the No-Three-In-Line problem.
2. Integrate UDEs to learn unknown energy dynamics (E) and learning loss $\mathcal{L}(\theta; x(t))$.
3. Perform simulations on the coupled UDE system.

7 Immediate Action Items

1. Implement the No-Three-In-Line model structure in Julia.
2. Create synthetic datasets of collinear triplets $\mathcal{L}$ for various grid sizes.
3. Replace the energy term E and learning loss $\mathcal{L}(\theta; x(t))$ with neural networks to form a UDE system.
4. Train the model using random initial conditions and perform forecasting.
5. Maintain a GitHub repository to store all code, trained models, and experiment logs.
6. The manuscript for this project is being written in Overleaf and can be accessed here.