

Interpretable Convolutional Kernels for Physical Principles Discovery from Observational Data

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Abstract

This paper presents a novel approach for learning complex physical principles from observational data using multi-scale group equivariant convolutional neural networks. We demonstrate the effectiveness of our method on two paradigmatic systems: Conway’s Game of Life cellular automata. Our neural architecture successfully discovers the underlying dynamical rules governing these systems by learning appropriate mapping functions that capture both local and long-range spatial interactions across multiple scales.

Keywords: Lattice Dynamics, Multi-Scale Group Equivariant Convolutional Neural Networks, Physical Principles, Dynamical Systems, Group representation theory

1 Introduction

Recent advances in deep learning, specifically convolutional neural networks, have shown remarkable promise in modeling spatial patterns and discovering underlying physical principles from data (?). Meanwhile, complementary work in symbolic regression has shown remarkable success in discovering explicit mathematical expressions from data, with AI Feynman and AI Feynman 2.0 successfully recovering all equations from the Feynman Lectures on Physics through physics-inspired techniques and Pareto-optimal symbolic regression (??). In molecular dynamics, the Deep Potential Molecular Dynamics (DeePMD) method has demonstrated how deep neural networks can learn many-body interatomic potentials from ab initio data while preserving essential physical symmetries (translation, rotation, and permutation invariance), achieving quantum mechanical accuracy at linear computational cost scaling (?).

In this work, we extend these ideas by developing a multi-scale convolutional neural network architecture specifically designed for learning complex physical principles from observational data. Our approach leverages the connection between convolution kernels and differential operators to automatically discover the governing equations of dynamical systems without prior knowledge of their mathematical form. We demonstrate the effectiveness of our method on ...

2 Problem Formulation

2.1 Lattice Field

Consider a discrete field system defined on a d -dimensional regular lattice $\Lambda \subset \mathbb{Z}^d$ (?). For each lattice site $\mathbf{i} = (i_1, i_2, \dots, i_d) \in \Lambda$, we define a field variable $\phi_{\mathbf{i}}(t) \in \mathcal{S}$, where \mathcal{S} represents the state space. The system’s configuration space can be expressed as:

$$\Phi(t) = \{\phi_{\mathbf{i}}(t) : \mathbf{i} \in \Lambda\} \in \mathcal{S}^{|\Lambda|} \quad (1)$$

This formulation naturally extends classical statistical mechanics to discrete lattice systems, where the fundamental principles of equilibrium and non-equilibrium dynamics can be rigorously analyzed (?).

The temporal evolution of the system is described by an operator $\mathcal{T} : \mathcal{S}^{|\Lambda|} \rightarrow \mathcal{S}^{|\Lambda|}$:

$$\Phi(t+1) = \mathcal{T}[\Phi(t)] \quad (2)$$

where the operator \mathcal{T} must satisfy the following fundamental constraints:

Locality Condition: The evolution of each lattice site depends only on its finite neighborhood:

$$\phi_{\mathbf{i}}(t+1) = f_{\text{local}}(\{\phi_{\mathbf{j}}(t) : \mathbf{j} \in \mathcal{N}(\mathbf{i})\}) \quad (3)$$

where $\mathcal{N}(\mathbf{i})$ denotes the neighborhood of lattice site \mathbf{i} .

Causality Condition: Information propagation has finite speed, i.e., there exists $v_{\text{max}} < \infty$ such that:

$$\text{supp}(\mathcal{T}^n[\delta_{\mathbf{i}}]) \subset B_{\mathbf{i}}(nv_{\text{max}}) \quad (4)$$

2.2 Physical Symmetry Principles

2.2.1 Time Translation Invariance

The evolution rules are independent of the choice of absolute time origin. Formally, for any temporal shift $\tau \in \mathbb{Z}$:

$$\mathcal{T}[\Phi(t)] = \Phi(t+1) \Leftrightarrow \mathcal{T}[\Phi(t+\tau)] = \Phi(t+\tau+1) \quad (5)$$

This is equivalent to requiring that the parameters of evolution operator \mathcal{T} contain no explicit time dependence.

2.2.2 Spatial Symmetry Group

Translation Invariance: For any lattice translation $\mathbf{a} \in \mathbb{Z}^d$, define the translation operator $T_{\mathbf{a}}$:

$$[T_{\mathbf{a}}\Phi]_{\mathbf{i}} = \Phi_{\mathbf{i}+\mathbf{a}} \quad (6)$$

The evolution operator commutes with translation operators:

$$\mathcal{T} \circ T_{\mathbf{a}} = T_{\mathbf{a}} \circ \mathcal{T} \quad (7)$$

Point Group Symmetries: For square lattices, the system exhibits C_{4v} point group symmetry, including:

- 90° rotational invariance: $\mathcal{T} \circ R_{\pi/2} = R_{\pi/2} \circ \mathcal{T}$
- Reflection invariance: $\mathcal{T} \circ \sigma = \sigma \circ \mathcal{T}$

2.2.3 Markovian Property and Information-Theoretic Structure

The system satisfies the strict Markov condition:

$$P(\Phi(t+1)|\Phi(t), \Phi(t-1), \dots, \Phi(0)) = P(\Phi(t+1)|\Phi(t)) \quad (8)$$

This implies that the system's "memory" is completely encoded in the current state, with no hidden historical dependencies.

2.2.4 Reversibility and Time-Reversal Symmetry

For conservative systems, the evolution operator is invertible, i.e., there exists an inverse operator \mathcal{T}^{-1} :

$$\mathcal{T}^{-1} \circ \mathcal{T} = \mathcal{T} \circ \mathcal{T}^{-1} = \mathcal{I} \quad (9)$$

This ensures that no information is lost in the system, and trajectories are deterministic in phase space.

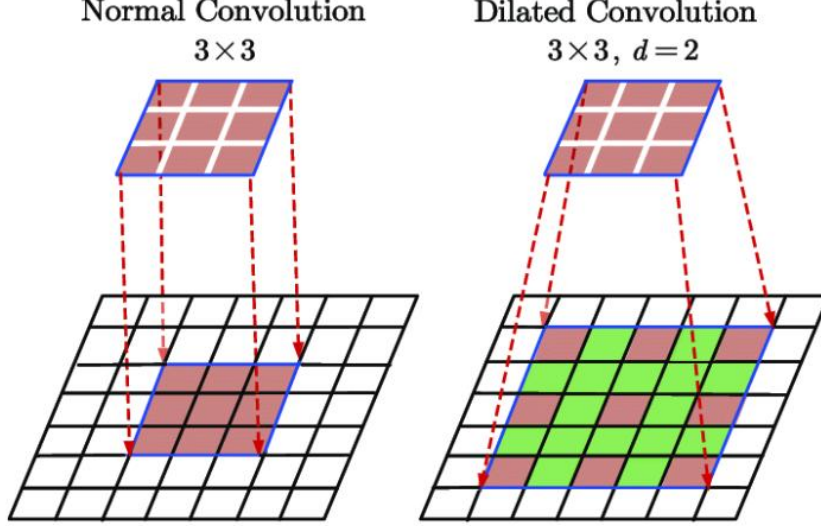


Figure 1: Multi-scale convolution operations for capturing spatial interactions at different scales.

3 Multi-Scale Convolutional Neural Networks

In this work, we use Multi-Scale Convolutional Neural Networks to discover the underlying physical principles governing dynamical systems by learning the mapping function \mathcal{F} that captures both local and long-range spatial interactions. The multi-scale architecture is essential because physical processes in spatiotemporal systems often involve interactions across multiple spatial scales simultaneously, from immediate neighbor effects to global pattern formation mechanisms.

Based on the aforementioned symmetry principles, our multi-scale CNN architecture should satisfy:

1. **Parameter Sharing:** Enforces translation invariance
2. **Equivariant Network Structure:** Preserves rotational and reflection symmetries
3. **Causal Convolution:** Ensures locality and causality constraints
4. **Time-Independent Parameterization:** Embodies time translation invariance

This structured inductive bias enables the network to efficiently learn physically reasonable dynamical rules while significantly reducing the required amount of training data.

4 Numerical Experiments

4.1 Conway’s Game of Life Rules

Let $\mathcal{G} \subset \mathbb{Z}^2$ be a finite 2D grid of size $H \times W$, where each cell $(i, j) \in \mathcal{G}$ has a binary state $s_{i,j}^{(t)} \in \{0, 1\}$ at discrete time $t \in \mathbb{N}$. The cellular automaton state at time t is defined as:

$$\mathbf{S}^{(t)} = \{s_{i,j}^{(t)} : (i, j) \in \mathcal{G}\} \in \{0, 1\}^{H \times W} \quad (10)$$

The evolution of the cellular automaton follows a deterministic update rule:

$$\mathbf{S}^{(t+1)} = f(\mathbf{S}^{(t)}) \quad (11)$$

where $f : \{0, 1\}^{H \times W} \rightarrow \{0, 1\}^{H \times W}$ is the global transition function.

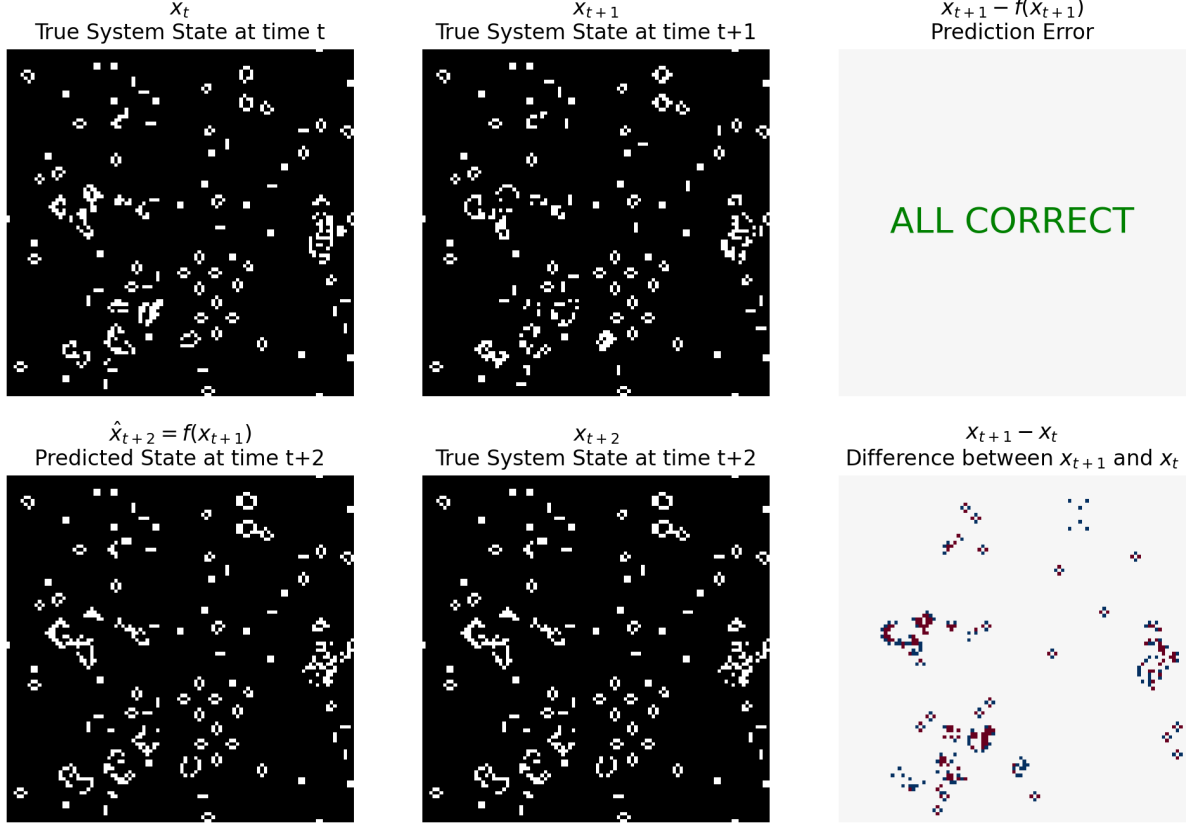


Figure 2: Multi-Scale Convolutional Neural Networks prediction accuracy for cellular automaton dynamics. Top row shows the system evolution from time t to $t + 1$, with perfect prediction accuracy. Bottom row demonstrates prediction at time $t + 2$. The right panels display prediction errors (top) and state differences between consecutive time steps (bottom).

For Conway’s Game of Life, the local transition rule for each cell (i, j) is defined as:

$$s_{i,j}^{(t+1)} = \begin{cases} 1 & \text{if } s_{i,j}^{(t)} = 1 \text{ and } n_{i,j}^{(t)} \in \{2, 3\} \\ 1 & \text{if } s_{i,j}^{(t)} = 0 \text{ and } n_{i,j}^{(t)} = 3 \\ 0 & \text{otherwise} \end{cases} \quad (12)$$

where $n_{i,j}^{(t)} = \sum_{(u,v) \in \mathcal{N}_{i,j}} s_{u,v}^{(t)}$ is the number of living neighbors in the Moore neighborhood:

$$\mathcal{N}_{i,j} = \{(i + \delta_i, j + \delta_j) : \delta_i, \delta_j \in \{-1, 0, 1\}, (\delta_i, \delta_j) \neq (0, 0)\} \quad (13)$$

From Fig.??, , we can observe that the multi-scale CNN architecture successfully learns the Conway’s Game of Life dynamics with remarkable accuracy. The model maintains high fidelity even for two-step ahead prediction $t + 2$, showing only minimal prediction errors scattered across a few isolated regions. The predicted state at $t + 2$ closely matches the true system evolution. From Figure.??, we can observe that the learned rules closely approximate the true Conway’s Game of Life dynamics. In the “dead to living” transition, predictions are almost exclusively concentrated at exactly 3 neighbors, precisely matching the birth rule. For “living to living” transitions, predictions are predominantly concentrated at 2 and 3 neighbors, perfectly aligning with the survival rule. The “dead to dead” and “living to dead” distributions demonstrate correct patterns for cell death or stasis under non-survival conditions, with prediction frequencies exhibiting exponential decay at incorrect neighbor counts.

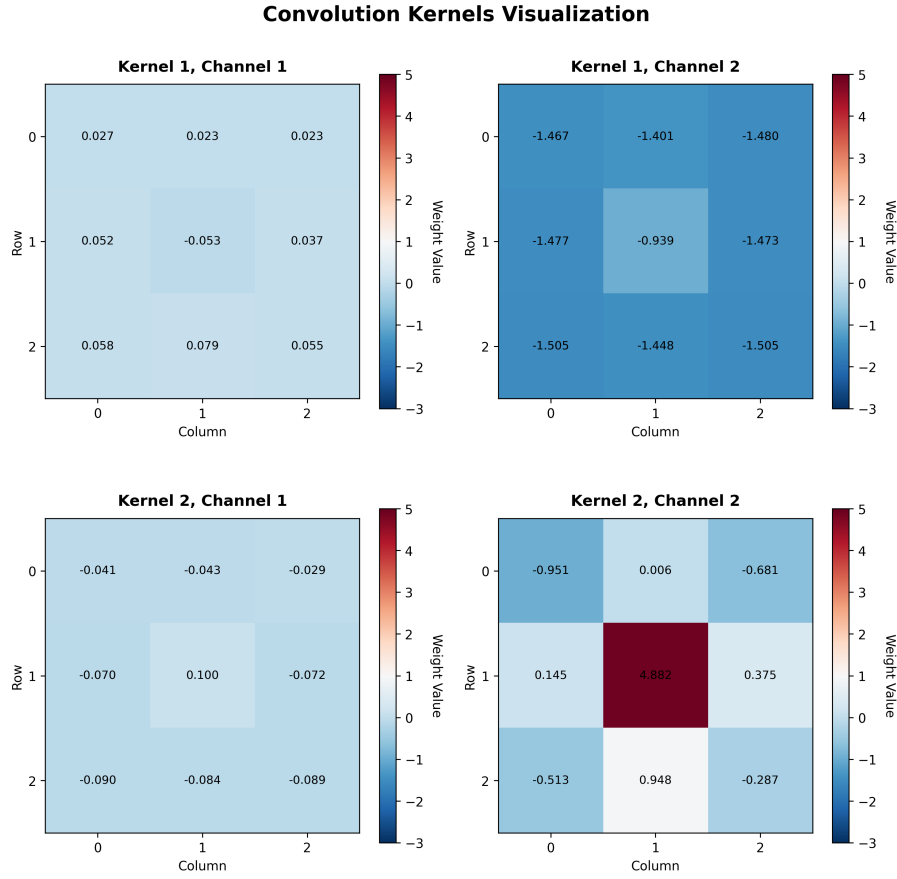


Figure 3: Visualization of learned convolution kernels of 1st layer in dataset with rule B3/S23

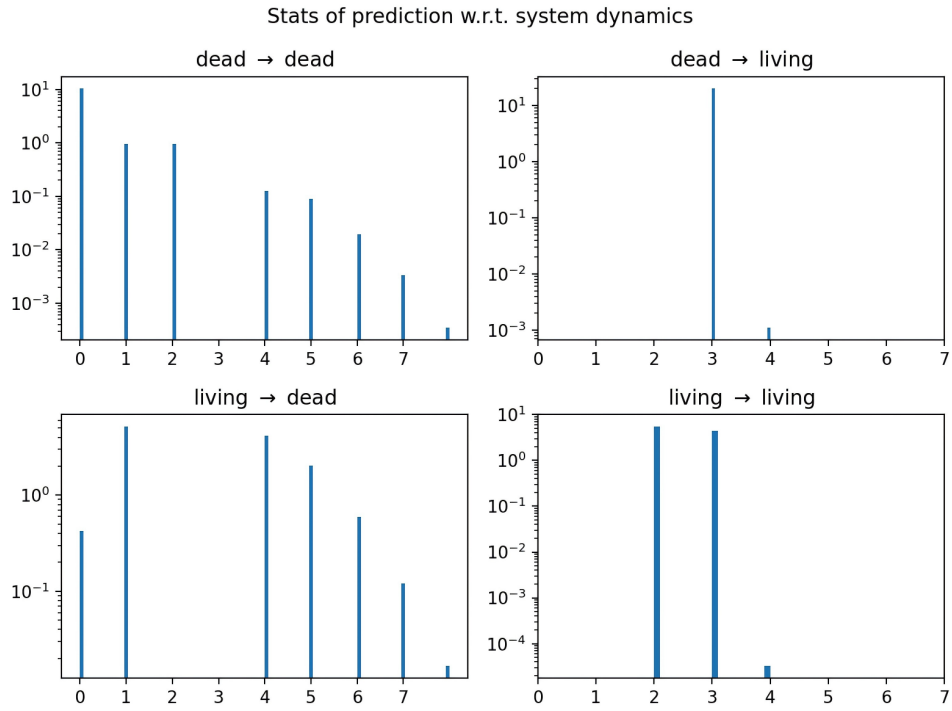


Figure 4: Learned cellular automaton rules.

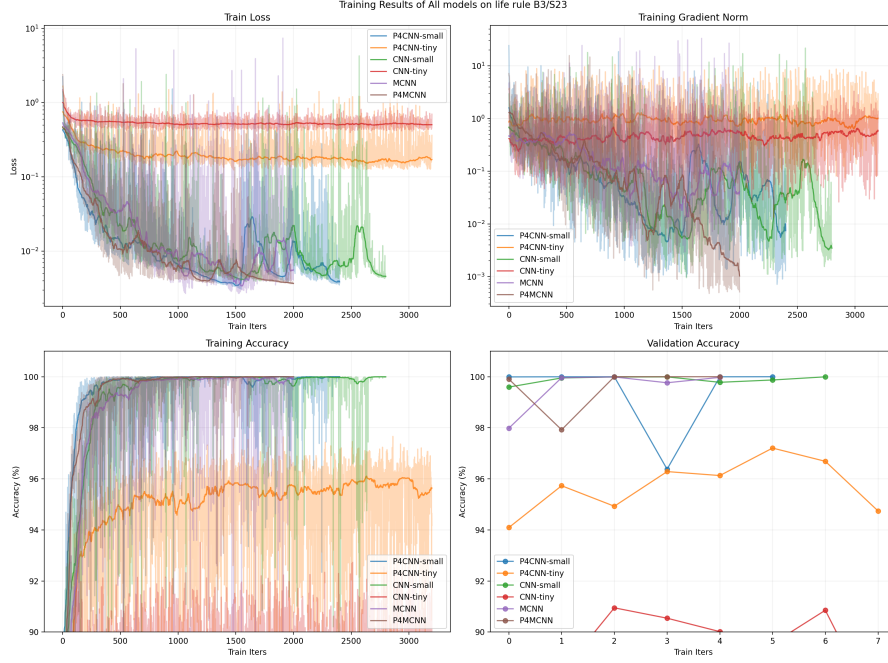


Figure 5: Training curves of different network architectures on dataset with rule B3/S23

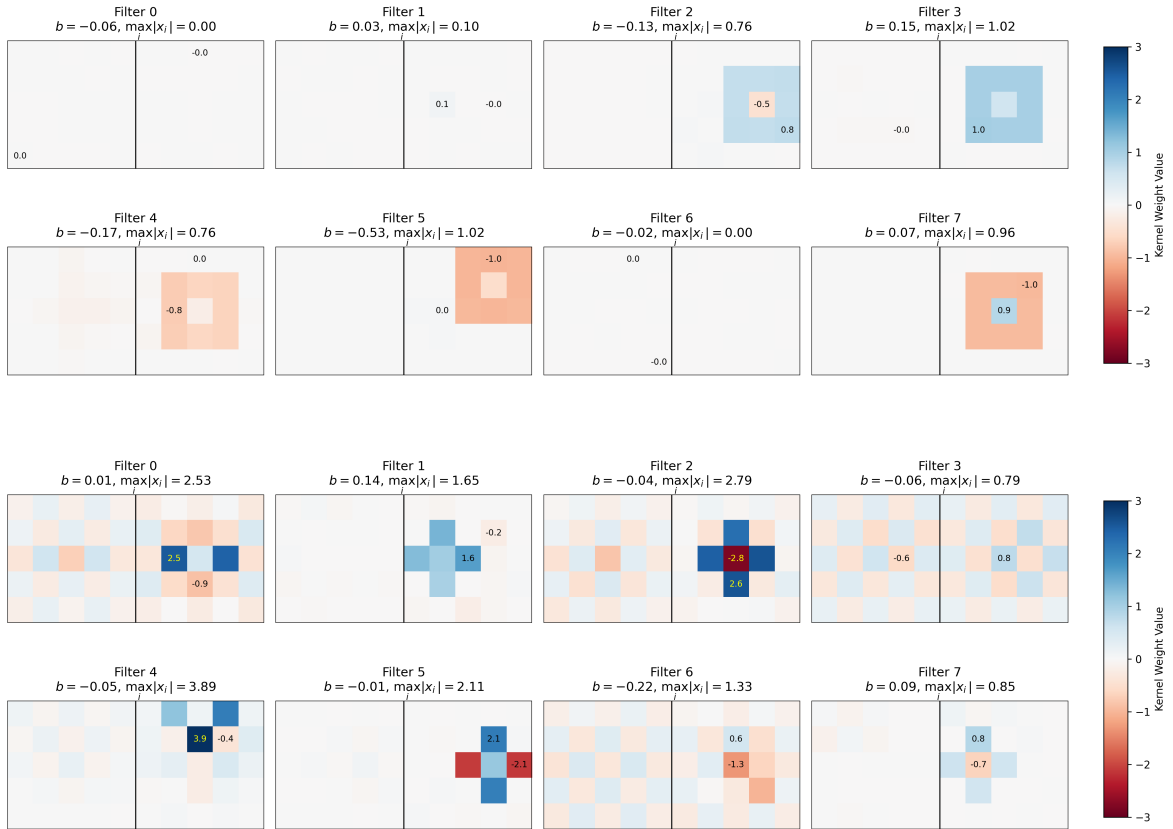


Figure 6: Trained convolution kernel weights of the 1st layer on dataset with rule B2/S (Up) and B13/S012V (Down)

Figure 7: Counting statistics of network-learned dynamics on whole dataset

Figure 8: Counting statistics of network-learned dynamics on whole dataset