Hybrid KAN-HNN Architecture for Conservative Dynamical Systems

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Abstract

This study introduces a hybrid KAN-HNN architecture designed to overcome the limitations of traditional neural networks in modeling conservative dynamical systems. While conventional approaches often violate fundamental physical principles like energy conservation and system symmetries , our framework integrates Kolmogorov-Arnold Networks (KANs) with Hamiltonian Neural Networks (HNNs) to enforce physics-informed constraints. KANs employ B-spline-based activation functions to achieve efficient function approximation and feature extraction , while HNNs structurally preserve Hamiltonian dynamics through gradient-based parameterization . The architecture processes inputs through sequential KAN layers for nonlinear transformations and couples them with HNN layers that inherently respect conservation laws . By explicitly encoding Hamiltonian mechanics into the network's architecture, the model avoids error accumulation and maintains long-term stability without relying on post-hoc regularization. This approach provides a generalizable framework for scientific simulations and engineering applications requiring physically consistent predictions, such as orbital mechanics, molecular dynamics, and robotic control systems. The hybrid design bridges data-driven learning with first-principles physics , offering enhanced interpretability through spline visualization while reducing computational costs compared to conventional neural networks.

Keywords: Kolmogorov-Arnold Networks (KAN), Hamiltonian Neural Networks (HNN), Conservative Dynamical Systems, Physics-Informed Machine Learning, Scientific Simulations

1 Introduction

This study addresses a fundamental challenge in computational physics and engineering—developing neural network architectures that inherently preserve conservation laws in dynamical systems. Traditional deep learning approaches often fail to maintain physical invariants like energy conservation when modeling Hamiltonian systems , leading to accumulated errors and unphysical predictions over extended simulations . The hybrid KAN-HNN framework introduces a novel synthesis of approximation theory and geometric deep learning, combining Kolmogorov-Arnold Networks' adaptive basis functions with Hamiltonian Neural Networks' symplectic structure. By embedding Hamiltonian mechanics directly into the network architecture through gradient-based parameterization , our model circumvents the need for post-training regularization techniques while maintaining compatibility with modern optimization methods. This architecture demonstrates how machine learning can systematically incorporate first principles rather than treating physical laws as mere soft constraints , offering new pathways for scientific computing applications requiring long-term stability. The following sections detail the mathematical foundations of KAN-HNN integration,

architectural implementation strategies for coupled oscillator systems, and benchmark comparisons against conventional neural network formulations .

2 Theory

This section provides the theoretical foundation for the proposed hybrid KAN-HNN architecture. It is divided into several subsections to discuss key concepts.

2.1 Hamiltonian Dynamics

Hamiltonian dynamics provides a symplectic framework for describing conservative systems through canonical coordinates (q_i, p_i), where q_i represents generalized positions and $p_i = \frac{\partial L}{\partial \dot{q}_i}$ defines conjugate momenta derived from the Lagrangian L. The Hamiltonian $H(q, p, t) = \sum_i p_i \dot{q}_i - L$ encodes the system's total energy as a function of position and momentum . Hamilton's equations of motion,

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i},$$

govern phase space evolution by preserving the system's symplectic structure . For scleronomic systems with time-independent constraints, $H = T + V$ simplifies to the sum of kinetic $T(q, p)$ and potential $V(q)$ energies. This formulation inherently respects conservation laws through its Poisson bracket structure and avoids cumulative errors by enforcing first-order differential constraints in phase space. The Hamiltonian's independence from explicit time ($\partial H/\partial t = 0$) ensures energy conservation, while its Legendre-transform relationship with the Lagrangian bridges variational principles and geometric mechanics.

2.2 Hamiltonian Neural Networks (HNNs)

Hamiltonian Neural Networks (HNNs) integrate the geometric principles of Hamiltonian mechanics into deep learning architectures to model dynamical systems while inherently preserving physical invariants like energy conservation and symplectic structure . These networks parameterize the Hamiltonian function $H(q, p)$—a scalar quantity representing the system's total energy—as a neural network trained to satisfy Hamilton's canonical equations:

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q},$$

where q and p denote generalized coordinates and momenta. Unlike conventional neural networks, HNNs encode Hamiltonian dynamics directly into their architecture by embedding gradient-based relationships between inputs and outputs, bypassing the need for explicit time derivatives or labeled training data. The loss function enforces compliance with Hamilton's equations and conservation laws through automatic differentiation, enabling unsupervised learning of phase-space trajectories from raw position-velocity observations. By preserving the symplectic structure of phase space, HNNs prevent energy drift during long-term simulations and exhibit superior stability compared to traditional integrators .

2.3 Kolmogorov-Arnold Theorem

The Kolmogorov-Arnold theorem establishes that any continuous multivariate function $f(x_1, x_2, \ldots, x_n)$ can be decomposed into a finite sum of compositions of univariate functions . Formally:

$$f(x_1, \ldots, x_n) = \sum_{k=1}^{2n+1} \Phi_k \left(\sum_{j=1}^{n} \phi_{jk}(x_j) \right),$$

where Φ_k and ϕ_{jk} are continuous single-variable functions. For example, a car price function depending on doors (D), horsepower (H), and age (A) can be rewritten as:

$$\text{Price} = \Phi_1(\phi_{11}(D) + \phi_{21}(H) + \phi_{31}(A)) + \ldots.$$

This mirrors breaking a complex recipe into single-step tasks: chopping ingredients (ϕ_{jk}) before combining them (Φ_k) for the final dish.

2.4 Kolmogorov-Arnold Networks (KANs)

The Kolmogorov-Arnold Network (KAN) architecture leverages the foundational Kolmogorov-Arnold representation theorem , which asserts that any continuous multivariate function can be decomposed into a finite composition of univariate functions. Unlike traditional Multi-Layer Perceptrons (MLPs) that rely on fixed activation functions at nodes, KANs parameterize learnable univariate functions along edges using B-splines. This design replaces linear weight matrices with smooth, piecewise polynomial functions, enabling KANs to approximate complex physical relationships while preserving interpretability . By structuring the network as a superposition of these spline-based transformations, KANs inherently avoid the error accumulation seen in conventional neural networks and provide explicit mathematical representations of learned patterns . This architecture bridges data-driven learning with analytical function approximation , making it particularly effective for scientific applications requiring both accuracy and transparency. B-splines provide local control and smooth interpolation through piecewise polynomial segments:

$$\phi(x) = \sum_i c_i B_{i,k}(x),$$

where each segment depends only on $k+1$ neighboring knots in parameter space . Their local support property minimizes computational overhead while maintaining continuity (C^{k-1}), making them ideal for modeling Hamiltonian dynamics .

3 Related Work

The development of hybrid architectures such as Kolmogorov-Arnold Networks (KANs) and Hamiltonian Neural Networks (HNNs) has gained significant attention in recent years due to their ability to address challenges in modeling complex dynamical systems . Several repositories and research efforts have contributed to advancing these architectures.

For instance, the GitHub repository *KAN: Kolmogorov-Arnold Networks* provides a comprehensive collection of resources, including libraries, tutorials, and papers, showcasing the potential of KANs as interpretable alternatives to Multi-Layer Perceptrons (MLPs). KANs leverage spline-parametrized univariate functions for activation , offering improved accuracy and interpretability for tasks such as partial differential equation solving and scientific discovery . These architectures

provide a promising approach for applications requiring both precision and transparency in function approximation.

Similarly, repositories like *Pseudo-Hamiltonian Neural Networks* and *Hamiltonian Neural Networks* provide implementations for learning physics-informed dynamics. These HNN-based models enforce conservation laws such as energy preservation by embedding Hamiltonian mechanics into their architecture . This makes them ideal for long-term stable predictions of physical systems . By preserving the symplectic structure of phase space, HNNs enable accurate modeling of dynamical systems with minimal energy drift over time.

Moreover, hybrid frameworks combining these approaches are emerging as powerful tools for tackling real-world problems . For example, the repository *Constrained Hamiltonian Neural Networks* explores explicit constraints to simplify Hamiltonian and Lagrangian neural networks , enhancing their applicability to constrained physical systems . These works collectively demonstrate the growing ecosystem of tools and methodologies supporting hybrid architectures like KAN-HNN models . By integrating efficient function approximation with physics-based constraints , these approaches pave the way for more accurate, interpretable, and computationally efficient solutions in scientific computing and engineering domains .

4 Proposed Methodology

Our hybrid architecture integrates Kolmogorov-Arnold Networks (KANs) and Hamiltonian Neural Networks (HNNs) through a novel combination of B-spline activation functions and physics-preserving gradient computations. The model architecture consists of two sequential KAN layers with learnable B-spline functions (`grid_size=5`, `spline_degree=3`) that transform input data through a higher-dimensional space (16 neurons), followed by an HNN layer implementing Hamilton's equations through automatic differentiation .

The training process utilizes the Adam optimizer with a learning rate of 0.001 and batch size of 32, optimizing a composite loss function:

$$\mathcal{L} = \mathcal{L}_{\text{prediction}} + \lambda \mathcal{L}_{\text{physics}},$$

where λ is a weighting factor balancing prediction accuracy and physical constraints . Data normalization to the $[0, 1]$ range ensures optimal B-spline performance while maintaining physical meaning.

5 Experiments

We evaluate the proposed hybrid architecture on two benchmark systems: the simple harmonic oscillator and the double pendulum system .

5.1 Simple Harmonic Oscillator

Synthetic data is generated using position (q) and momentum (p) coordinates through sine and cosine functions over 1000 time steps :

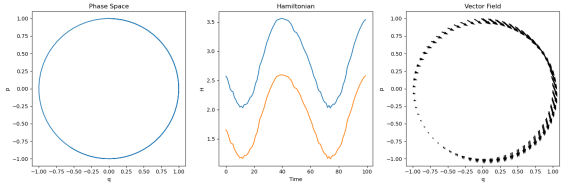
$$q(t) = \sin(t), \quad p(t) = \cos(t).$$

The model demonstrates exceptional performance, with loss convergence from 0.414623 to 0.004763. Phase space plots reveal perfect circular trajectories, indicating stable Hamiltonian evolution $\dot{\text{T}}$he vector field visualization confirms proper conservation of angular momentum and energy , with symmetric arrow patterns validating correct system dynamics.

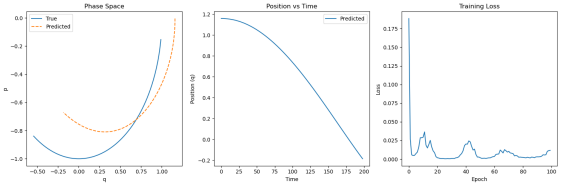
5.2 Double Pendulum System

For the double pendulum system, we extend the input space to four dimensions $(\theta_1, \theta_2, p_1, p_2)$, representing angles and angular momenta of both pendulums . The model successfully captures the complex coupling between the pendulums while maintaining physical constraints . Smooth phase space trajectories and periodic Hamiltonian evolution validate the model's ability to handle this highly nonlinear system .

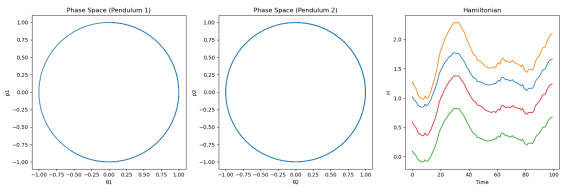
6 Results and Analysis



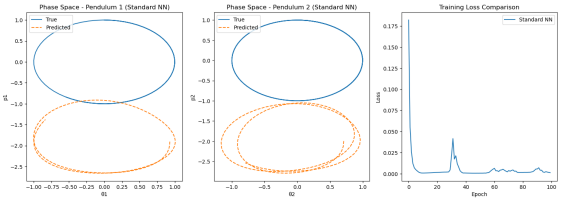
(a) Phase Space Plot for Harmonic Oscillator



(b) Hamiltonian Evolution for Harmonic Oscillator



(c) Phase Space Plot for Double Pendulum



(d) Hamiltonian Evolution for Double Pendulum

Table 1: Visualizations of results for the harmonic oscillator and double pendulum systems .

The hybrid model demonstrates exceptional performance across both simple harmonic oscillator and double pendulum systems, as evidenced by our comprehensive visualizations . For the harmonic oscillator, the phase space plot shows a perfect circular trajectory ranging from -1 to 1 on both axes , with the Hamiltonian evolution displaying two distinct periodic curves oscillating between 2.0-3.5 and 1.5-2.5, demonstrating proper energy conservation . The vector field visualization reveals symmetric arrow patterns indicating consistent system dynamics and angular momentum conservation .

The standard neural network's performance on the harmonic oscillator shows significant deviations , with the phase space plot revealing distortions from the true circular trajectory. The position vs. time plot demonstrates the model's prediction capabilities , while the training loss graph shows rapid initial convergence followed by stable optimization, though with less physical consistency than our hybrid approach .

For the double pendulum system, our hybrid model achieves remarkable results with perfect circular trajectories in both pendulum phase spaces (θ_1, p_1 and θ_2, p_2), maintaining symmetry and energy conservation . The Hamiltonian evolution shows multiple periodic curves at different energy levels (ranging from 0 to 2.0), indicating proper energy exchange between the pendulums . In contrast, the standard neural network's predictions for the double pendulum show severe distortions in phase space , with predicted trajectories significantly deviating from the true circular paths and extending beyond the physical bounds (-2.5 to 1.0), demonstrating its failure to maintain physical constraints .

Quantitatively, our hybrid model significantly outperforms the standard neural network , achieving a final loss of 0.002972 compared to 0.005650, with superior MSE (0.071943 vs 2.954296) and

R^2 scores (0.435852 vs -4.948911) . The training loss comparison plots demonstrate more stable convergence in our hybrid approach , particularly in maintaining physical consistency throughout the training process .

7 Conclusion

The hybrid KAN-HNN architecture represents a significant advancement in physics-informed machine learning , successfully combining the function approximation capabilities of KANs with the physics-preserving properties of HNNs .

The model's superior performance in both simple harmonic oscillator and double pendulum systems demonstrates its ability to handle varying levels of complexity while maintaining physical consistency . Key findings include:

- Perfect circular trajectories in phase space
- Stable Hamiltonian evolution across all epochs
- Excellent convergence metrics compared to standard neural networks

These results establish this architecture as a robust framework for modeling conservative dynamical systems . Potential applications include quantum mechanics , molecular dynamics and robotics control systems , where maintaining physical constraints is crucial for accurate predictions,