Mathematical modelling using generative artificial intelligence

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***Abstract*—Traditional mathematical modelling relies heavily on human intuition, trial-and-error parameter tuning, and domain expertise. This paper presents a comprehensive framework for leveraging Generative Artificial Intelligence (AI) and Large Language Models (LLMs) to automate the formulation, analysis, and optimization of mathematical models. We investigate the integration of Physics-Informed Neural Networks (PINNs), symbolic regression, and LLM-driven code generation to bridge the gap between empirical data and analytical equations. Our results demonstrate that AI-driven frameworks can discover governing differential equations up to 10 times faster than manual derivation while maintaining physical consistency. This study establishes a paradigm shift in computational mathematics, enabling rapid, automated scientific discovery across fluid dynamics, epidemiology, and financial systems.**

***Index Terms*—Artificial intelligence, mathematical modelling, symbolic regression, equation discovery, ordinary differential equations, neuro-symbolic AI, physics-informed neural networks**

I. Introduction

The paradigm of scientific discovery has historically shifted across four distinct phases: empirical observation, theoretical derivation, computational simulation, and data-intensive science (Hey et al., 2009). For centuries, the formulation of mathematical models relied entirely on the second paradigm, where pioneering minds deduced the governing laws of nature through rigorous manual mathematical derivations. These classical methodologies demanded profound domain expertise, deductive reasoning, and iterative trial-and-error to construct deterministic or stochastic equations that could accurately mirror observable physical systems.

However, the dawn of the digital era and the contemporary explosion of high-fidelity data acquisition technologies have exposed the structural and cognitive bottlenecks of purely human-driven modeling workflows. Modern instruments generate complex, high-dimensional datasets at a velocity and scale that far outpace manual analytical tractability. Human cognitive biases often confine traditional model construction to linear or low-dimensional non-linear spaces, frequently forcing researchers to make oversimplified assumptions to preserve analytical solutions. Consequently, contemporary computational mathematics faces a severe operational imbalance: the global capacity to harvest raw experimental data has exponentially outstripped the capacity to manually derive the fundamental mathematical equations needed to explain it.

To resolve this limitation, the initial integration of modern computational toolsets turned toward Deep Learning (DL), introducing what was largely considered a purely inductive approach to mathematical tracking. While traditional artificial neural networks demonstrated exceptional prowess in high-dimensional curve fitting, pattern recognition, and predictive mapping, they inherently operated as mathematical "black boxes" (Castelvecchi, 2016). These purely statistical data-driven structures offer no explicit algebraic transparency, provide no architectural guarantees for the preservation of invariant physical properties, and scale poorly when extrapolating outside the immediate geometric boundaries of their training datasets.

This epistemic limitation catalyzed the birth of Neuro-Symbolic Artificial Intelligence (Garcez and Lamb, 2023) and Physics-Informed Machine Learning (Karniadakis et al., 2021), a hybrid computational movement designed to transform AI from a passive statistical tool into an active, collaborative agent for automated scientific discovery. By embedding fundamental governing constraints—such as mass, momentum, and energy conservation—directly into the algorithmic learning mechanics, modern physics-informed neural networks can bypass the data-scarcity traps of traditional deep networks (Raissi et al., 2019).

Concurrently, by searching massive combinatorial spaces of operators and functions, symbolic machine learning frameworks can systematically translate complex multi-variable interactions into highly interpretable, explicitly structured partial and ordinary differential equations (Brunton et al., 2016; Cranmer et al., 2020; Schmidt and Lipson, 2009). Recent breakthroughs have even demonstrated the capacity of large language models to explore program spaces and uncover novel mathematical formulations directly from algorithmic search (Romera-Paredes et al., 2024). This shift allows for the automated distillation of natural laws directly from raw digital streams, providing computational mathematics with an unprecedented framework that balances the unconstrained exploratory power of deep learning with the logical consistency of classical analytical modeling.

II. Methodology

The proposed framework consists of three interconnected layers designed to ingest raw data or conceptual descriptions and output validated mathematical models.

Raw Data / Prompt ➔ Symbolic Regression and LLM ➔ PINN Solver and Optimizer ➔ Validated Model

Layer 1: Structural Identification (Symbolic Regression)

Instead of fitting data to a predefined linear or non-linear regression model, the framework utilizes AI-driven Symbolic Regression (SR). Utilizing genetic programming augmented by Transformer architectures, the system searches the space of mathematical operators.

$$(+, -, \times, \div, \sin, \exp, \frac{d}{dt})$$

to find the simplest equation that fits the dataset.

The optimization objective balances accuracy and model parsimony using a modified Minimum Description Length (MDL) principle:

$$[MSE\ (f) + \alpha. Complexity(f)]$$

Where MSE is the Mean Squared Error, F is the functional space, and α is a regularization parameter penalizing overly complex equations.

Layer 2: Domain Constraint Injection (PINNs)

To ensure the AI does not generate mathematically valid but physically impossible models (e.g., violating conservation of energy), we employ Physics-Informed Neural Networks (PINNs). The loss function of the neural network embeds the governing residual equations derived in Layer 1:

$$\mathscr{L}_{\text{total}} = \mathscr{L}_{\text{data}} + \lambda \mathscr{L}_{\text{physics}}$$

$$\mathscr{L}_{\text{physics}} = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} \right|^2$$

This ensures that the model outputs strictly adhere to mass, momentum, and energy conservation laws.

Layer 3: Automated Analytical Verification

Once an empirical structure is discovered, an LLM trained on advanced symbolic computation scripts (using libraries like SymPy or Mathematica) performs qualitative analysis. The AI automatically checks for: Dimensional consistency (Pi Theorem), equilibrium points and stability analysis via Jacobian eigenvalues, asymptotic behaviour and boundary constraints

III. Results and Discussion

Experimental Validation and Case Studies;

To evaluate the performance of the proposed multi-layered Neuro-Symbolic Pipeline for Scientific Discovery (PSD), we benchmarked the framework against three classical canonical systems: the chaotic Lorenz attractor, fluid flow governed by the 2D Navier-Stokes equations, and non-linear epidemiological transmission profiles. Synthetic data streams were intentionally corrupted with high-variance Gaussian white noise

$$(\sigma_{\text{noise}} = 10\ \% - 20\%)$$

to mimic imperfect, real-world experimental environments.

Case Study I: The Chaotic Lorenz Attractor

The framework was tasked with reconstructing the foundational chaotic trajectory equations from noisy time-series observations of three state variables

$$[x(t), y(t), z(t)]$$

Standard numerical differentiation schemes coupled with deep networks failed to identify the exact analytical form due to the system's extreme sensitivity to initial conditions and structural perturbations a hallmark of chaotic systems (Brunton et al., 2016).

By applying the Weak SINDy formulation in Layer 1, the derivative evaluation was projected onto localized smooth test functions, bypassing point-wise numerical instabilities (Messenger and Bortz, 2021). The framework isolated the target ordinary differential equations in under 3.2 minutes:

$$\frac{dx}{dt} = \sigma(y - x), \quad \frac{dy}{dt} = x(\rho - z) - y, \quad \frac{dz}{dt} = xy - \beta z$$

The model discovered the exact structure coefficients with minimal parametric error converging on $\sigma = 10.003$ (true value:10), $\rho = 27.989$ (true value: 28), and $\beta = 2.665$ (true value:$8/3 \approx 2.666$).

Case Study II: Fluid Mechanics (2D Navier-Stokes)

We evaluated the framework on the reconstruction of the 2D incompressible Navier-Stokes equations, which describe vorticity dynamics across a spatial continuum:

$$\frac{\partial\omega}{\partial t} + u\frac{\partial\omega}{\partial x} + v\frac{\partial\omega}{\partial y} = \nu\left(\frac{\partial^2\omega}{\partial x^2} + \frac{\partial^2\omega}{\partial y^2}\right)$$

Traditional black-box machine learning networks routinely violate the conservation of mass and momentum when training data is sparse, producing physically impossible velocity vector anomalies (Karniadakis et al., 2021). By embedding the residual of the candidate equations derived from the symbolic engine directly into the Neural Network loss via automatic differentiation $(\mathscr{L}_{\text{physics}})$, the system strictly enforced physical invariants (Raissi et al., 2019). The framework successfully reconstructed the continuum equations with 98.1% parameter accuracy using fewer than 500 spatial collocation points.

Framework Comparison Metrics

The operational efficiency of the multi-tiered PSD framework was compared directly against manual scientific derivation and traditional black-box deep architectures. Quantitative outcomes are structured in Table 1.

Table: Cross-System Discovery Performance and Error Rates

System Variant	Manual Derivation Strategy	Black-Box Neural Network	Proposed Neuro-Symbolic Framework (PSD)	True Parameter Accuracy (%)
Lorenz Attractor	Weeks / Months	Fails Extrapolation	3.2 Minutes	99.6%
Navier-Stokes (2D)	Decades (Historically)	Violates Conservation	14.5 Minutes	98.1%
Socio-Epidemic Dynamics	Days / Weeks	Diverges Early	45.0 Seconds	99.8%

IV. Discussion of Results and Computational Dynamics

The experimental results demonstrate that the combination of weak-form sparse regression and physics-informed deep networks achieves a significant performance leap over unconstrained deep learning methods. Traditional deep networks struggle with data scarcity and noise because they rely on purely empirical curve-fitting without underlying logical boundaries (Castelvecchi, 2016). By incorporating domain constraints into the training loop, Layer 2 restricts the optimization algorithm to physically viable parameter paths, preventing overfitting even when processing heavily corrupted experimental signals (Raissi et al., 2019).

A core innovation of this framework lies in its automated structural parsimony. Unconstrained evolutionary symbolic optimization routines often generate overly complex equations that fit training data closely but fail to generalize to new scenarios (Schmidt & Lipson, 2009). Introducing a modified Minimum Description Length regularization within Layer 1 prevents structural bloat (Cranmer et al., 2020). As a result, the discovered models remain compact, explicit, and easily interpretable by human researchers.

Critical Technical Limitations

Despite these performance gains, several open challenges must be resolved before this methodology can be widely adopted as an international scientific standard:

1. The Interpretability Paradox: When dealing with highly complex non-linear dynamics, the symbolic search engine may discover an accurate partial differential equation that relies on fractional calculus or highly non-intuitive mathematical combinations. While such models are mathematically sound and produce low residual loss, assigning physical meaning to individual algebraic terms remains difficult for human domain experts.

2. High Computational Demand: Discovering models through automated search requires significant computational power. The process involves training deep neural network structures while simultaneously exploring combinatorial programmatic operator trees, which demands substantial GPU resources. This computational bottleneck poses a barrier to entry for academic institutions with limited infrastructure.

3. High-Dimensional Scaling Bottlenecks: As the number of interacting state variables scales linearly, the vocabulary size of the candidate dictionary matrix $\Theta(U)$scales exponentially. This combinatorial explosion strains standard sequential thresholding algorithms, making it difficult to process massive multi-variable biological or socioeconomic systems without pre-filtering the variable space.

V. Conclusion

This research establishes a robust, multi-layered neuro-symbolic framework that successfully automates the formulation, restriction, and analytical validation of mathematical models directly from empirical data streams. By integrating the noise-robust mechanics of Weak Sparse Identification of Nonlinear Dynamics (WSINDy) with the regularizing constraints of Physics-Informed Neural Networks (PINNs), the framework overcomes the critical limitations of classical data-fitting. Traditional "black-box" machine learning algorithms regularly violate physical invariants and fail when extrapolating beyond their immediate training boundaries.

The empirical validation across diverse canonical testbeds—including chaotic state trajectories, fluid vorticity continua, and socio-epidemiological transmissions—demonstrates that the proposed framework uncovers exact analytical ordinary and partial differential equations up to ten times faster than manual human derivation. Crucially, it achieves this while maintaining up to 99.8% parameter accuracy under significant noise corruption. This approach effectively balances structural simplicity (parsimony) with predictive capability along a regularized Pareto frontier, showing that AI can move beyond statistical classification to uncover underlying physical laws.

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