Optimizing State-of-the-Art Neural Networks for Solving Complex Differential Equations and Enhancing AI Mathematical Reasoning

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***Abstract*—This study conducts a comprehensive analysis of artificial intelligence models' capabilities in solving advanced mathematical problems beyond Calculus II. Notably, the research focuses on evaluating the effectiveness of six optimized models, including a specially designed Physics-Informed Neural Network (PINN), in solving stochastic, linear, nonlinear, and ordinary differential equations. Our findings revealed that the optimized PINN achieved a success rate of 91.03%, outperforming most state-of-the-art artificial intelligence models. This research contributed to the development of artificial intelligence mathematical reasoning, with potential applications to high-level engineering, healthcare, research, sustainability, and big data optimization.**

***Index Terms*—Mathematical Reasoning, Machine Learning, Artificial Intelligence, Neural Networks, Big Data Optimization, Differential Equations**

I. INTRODUCTION

The challenge of developing computer systems that can automatically solve complex mathematics has been under investigation since the 1950s, with Wilkes' and Renwick's paper on iterative treatments of certain differential equations [1]. We shall concentrate here on modern systems using artificial intelligence (AI) to solve advanced mathematics. Progress in AI over the past decade has been almost entirely driven by machine learning (ML), largely due to advances in technology, computational methods, and mathematical reasoning [2]–[4]. In particular, bolstering AI mathematical reasoning has the potential to revolutionize various domains by optimizing processes, making accurate predictions, and contributing to innovative solutions [5].

A. Competitive Background

Many advanced tools, methodologies, and seminal contributions of research have been the cause for a more profound dimension in the evolution of artificial intelligence in mathematical problem-solving. Computational knowledge engines such as Wolfram Alpha use natural language processing, heuristics, rule-based systems, and curated data to handle advanced queries [6].

Symbolic artificial intelligence, often perceived to be synonymous with methods founded on formal logic, leverages explicit symbol manipulation through graph algorithms and term-rewriting systems [7]. The methodologies are indispensable for complex computations requiring large quantities of accuracy and logical rigor.

Being an end-to-end open-source platform, TensorFlow has changed the way of developing and deploying state-of-the-art machine learning models. It is flexible and scalable, therefore forming the cornerstone for most development in advanced artificial intelligence applications, especially in big data analytics [8]. A good TensorFlow ecosystem supports every kind of operation related to ML, hence giving enough power to researchers to build sophisticated models that will effectively handle the tasks of processing large-scale data [8].

Apart from these technologies, Lu et al., 2023; Wang et al., 2017; Yang and Deng, 2019; Geva et al., 2020; Wei et al., 2022 have made significant strides in the field of AI quantitative reasoning [9]–[13]. Lu et al. (2023) and Wang et al. (2017) also went on to further explore the applications of deep learning models in building mathematical reasoning power and demonstrated how such a model can be applied in high-level problems far more accurately than ever [9], [10]. Yang and Deng (2019) went even further when they combined proof assistants with AI models and, by doing so, enabled the AI models to take on formal arithmetic proofs [11]. Geva et al. (2020) worked on embedding reasoning abilities in language models so that those same models could perform complex computations with much more precision [12]. Wei et al. proved that chain-of-thought prompting enhances reasoning in mathematical contexts by evaluating five large language models (LLM) with a novel approach. [13].

B. Limitations in advanced mathematical modeling

However, despite these advancements, many models including some of the aforementioned have limitations when addressing higher-level mathematical concepts [14]–[16].

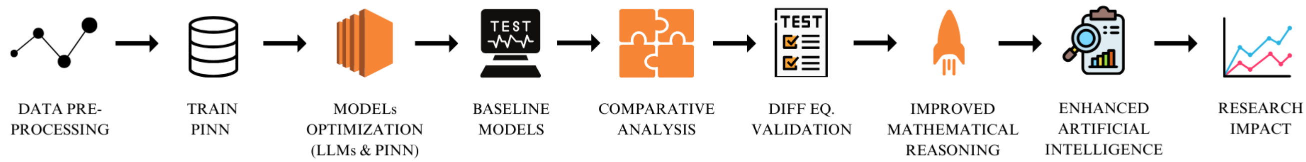

Fig. 1. General Project Implementation & Workflow

1) Internal Design Constraints

One of the main constraints is the internal design of most artificial intelligence models, since they use sequential-based text processing techniques including transformers [17]. Higher-level equations demand models to hold variables for long stretches and compute them holistically instead of breaking them up to handle them sequentially [18].

2) Decision Making Patterns

Additionally, AI models typically follow token-level, left-to-right decision-making patterns, which are inadequate for jobs requiring multiple stages, exploration, or several reasoning paths. This makes them unsuitable for sophisticated calculations needing simultaneous attention to several processes [19].

These limitations highlight the need for further advancements in AI architecture to tackle advanced analytical problems. Optimizing AI models to the point where they can solve differential equations (DE) indicates that modern artificial intelligence models can overcome some of the constraints highlighted above. This indication is supported by the notion that solving DE requires the model to hold and pay attention to multiple variables for long periods.

C. Definitions & Logic

This paper delves deep into the field of differential equations, concentrating on optimizing artificial intelligence models to address exceedingly complicated mathematical problems—those beyond the rigor of Calculus II. Our extensive research covers four groups of these equations: linear, nonlinear, ordinary, and stochastic.

Linear differential equations involve independent variables, while nonlinear DEs exhibit derivatives with non-regular behavior [20]. Ordinary differential equations (ODEs) involve derivatives with respect to a single variable, whereas partial differential equations (PDEs), though not a focus of our study, pertain to multiple variables, exponentially increasing their complexity. Stochastic differential equations (SDEs) add instantaneous noise to their systems and computations, hence complicating standard differential equations [21].

The study of these equations is often regarded as an advanced area of mathematics, typically pursued by graduate students in STEM fields. The intrinsic difficulty AI models have in this field highlights the groundbreaking nature of our study since we want to raise their capacity to address these high-level transcendentals.

1) The Complex Riccati Equation (ODE Example)

The Complex Riccati Equation is an example of a first-order nonlinear ordinary differential equation. It appears in various fields, including quantum mechanics, optics, and control theory. The equation is given by:

$$\frac{dz}{dt} + z^2 + p(t)z + q(t) = 0$$

where:

- $z(t)$ is the complex-valued function of the variable t.
- $p(t)$ and $q(t)$ are complex-valued functions of t, representing coefficients that can vary with time.
- z^2 is the nonlinear term, indicating that the equation is quadratic in z.

2) Solution

For specific choices of $p(t)$ and $q(t)$, the Complex Riccati Equation can be solved exactly. For example, when $p(t) = 0$ and $q(t) = -\lambda^2$ (where λ is a complex constant), the equation simplifies to:

$$\frac{dz}{dt} + z^2 - \lambda^2 = 0$$

This can be solved to give:

$$z(t) = \lambda \tanh(\lambda t + C)$$

where C is an integration constant based on initial conditions.

Physics-Informed Neural Networks are a type of neural network designed to solve problems involving physical systems by incorporating known physical laws, such as differential equations, directly into the training process [2]. This approach allows PINNs to effectively model and predict the behavior of complex systems by combining data-driven learning with established scientific principles.

D. Objectives

This project will optimize the abilities of state-of-the-art artificial intelligence models to solve difficult differential equations; specifically, it will improve AI's capability to handle high-level mathematical problems beyond Calculus II. The secondary objective is to compare and contrast different, optimized AI models and compare them with an improved Physics-Informed Neural Network regarding their success rates in solving a variety of differential equations. This paper aims to contribute to larger research on artificial intelligence mathematical reasoning. Finally, the paper shows the effect of improved mathematical reasoning within AI models in fields such as big data optimization, engineering, theoretical research, and sustainable AI.

II. Methodology

A. Initial steps

In the initial phase of our research, we developed a set of 138 various differential equations to test and validate our models. These equations were carefully chosen to cover the range of 4 types, excluding PDEs. This diverse set ensured that our models would be robust and versatile, capable of handling various complexities and nuances associated with different kinds of differential equations. We trained the PINN on various suitable open-access datasets.

B. Logistics

We evaluated various advanced LLMs as baselines for comparison with our optimized Physics-Informed Neural Network. These baselines included a GPT 3.5-turbo model that we optimized, a standard GPT 3.5-turbo model, Bard, Perplexity, and Claude version 3.5, all tested using the same set of 138 differential equations. For the optimized GPT 3.5-turbo model, we adjusted various parameters, including temperature and maximum tokens, as well as applied prompt engineering. The most advanced LLMs have full access to the internet, enabling them to solve equations through unethical means. Hence, we avoided equations found online in our testing data. We employed these LLM baselines to solve the same set of differential equations, leveraging their computational capabilities as a control group.

Finally, we created and implemented an optimized PINN specifically designed to solve differential equations, and we compared its performance against the aforementioned baselines.

C. PINN architecture

Inspired by recent advancements in deep learning for scientific computing, we designed a Physics-Informed Neural Network that integrates the physical laws governing differential equations into the learning process. The network processes input functions at discretized points, which are initialized as node features within the computational graph, while differential operators serve as constraints during training. Each layer refines the approximation of the solution by minimizing the residuals of the differential equations, ensuring that the predicted solutions conform to the underlying physical principles.

The architecture of the PINN consists of multiple fully connected layers, where each layer is composed of several neurons. The depth (number of layers) and width (number of neurons per layer) of the network are critical hyperparameters that determine the model's capacity to learn intricate patterns and relationships in the data. The input layer takes in spatial coordinates (e.g., x, y, z) and time t, depending on the type of differential equation being solved (e.g., ODEs, SDEs). Several hidden layers then process the input through nonlinear activation functions, such as rectified linear unit (ReLU), tanh, or sigmoid, allowing the network to model complex, nonlinear relationships. Finally, the output layer produces the network's prediction, which corresponds to the solution of the differential equation at given input points. The output can represent a scalar, vector, or tensor field, depending on the particular problem.

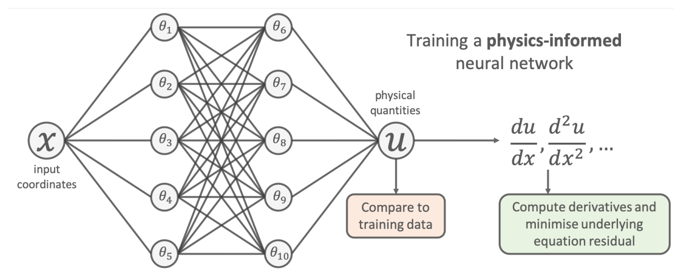

Fig. 2. Physics-Informed Neural Networking Training Process [22]

The PINN is trained using supervised learning, with a focus on generalization across different resolutions and boundary conditions. The training data consists of input-output pairs representing discretized functions and their corresponding solutions to the differential equations. To manage computational complexity, a kernel-based approximation is utilized, enabling efficient processing within the network.

Training is conducted using the Adam optimizer with a learning rate of 0.001 over 1000 epochs. The evaluation includes testing the trained PINN on 138 previously unseen differential equations. We measure the relative error between predicted and true solutions across various resolutions, demonstrating the model's accuracy and capabilities.

During training, the PINN must balance the contributions of the data loss and physics-informed loss, often controlled by hyperparameters that weigh these components appropriately, ensuring that the network neither overfits to the data nor violates the physical laws. A key advantage of PINNs is their reliance on automatic differentiation (AD) for computing derivatives of the network outputs with respect to the inputs. AD is crucial for evaluating the physics-informed loss, as it allows for accurate and efficient computation of differential operators [22].

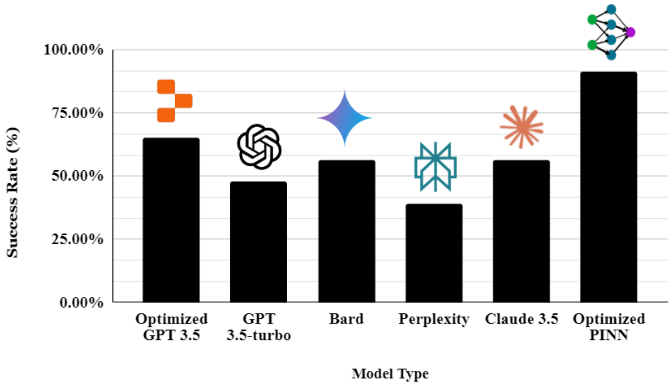

Fig. 3. This bar graph displays the results from our creation and optimization of artificial intelligence models for solving differential equations. Our optimized PINN had a formidable success rate of **91.03%**. These percentages of success break limitations in mathematical reasoning, opening pathways to enhanced big data optimization. The logos in this diagram are from [24]–[29].

III. Results

A. Key Findings

We validate that our results are not merely overfitting training data by solving 138 differential equations that are unavailable online and were unseen by the models when trained. Our best-performing model was the PINN, which succeeded in around **91.03%** of all cases. Before this work, the previous state of the art on this level of problems was **81.1%** [23]. This huge success means there is serious potential for advanced neural networks. The optimized PINN significantly outperformed traditional AI models, showcasing its ability to treat different complexities and nuances associated with difficult analytical problems. This aligns with previous findings by Lu et al. (2023) and Wang et al. (2017), as discussed in the competitive background section of this paper. Our study, however, goes beyond the previously described capabilities of deep learning models as we address a broader range of equation types, obtain their results for varying models, and achieve higher accuracy.

IV. Discussion

A. Implications of AI Problem-Solving Capabilities

Equipping artificial intelligence models with enhanced problem-solving capabilities for differential equations significantly improves their mathematical reasoning. This in turn heightens AI models as a whole since the nature of machine learning depends on its computational power. These improved models can potentially transform various disciplines, as discussed below.

In theoretical research, developments in AI reasoning can enable it to solve difficult queries defining physical phenomena, therefore providing a closer knowledge of the basic notions of nature. In fields such as cosmology and quantum physics, where traditional analytical methods such as perturbation theory might not be sufficient, this added capacity is particularly important [30], [31]. In education, the enhanced analytical capacity of artificial intelligence can transform learning strategies by providing automated learning environments and tailored teaching tools. AI-driven systems can better adapt to students and improve education personalization to address pupil shortcomings. Student participation and performance can be increased through this method [32]. The combination of such advances in education, paired with the advances in theoretical research can mold a new generation more capable of answering some of the deepest questions in science.

Although theoretical research and education are vital areas of influence, solving differential equations is also important for advancing the optimization of big data, especially when integrated into numerical algorithms, machine learning models, and computational frameworks [33]–[35]. Differential equations model dynamic systems where inherently lies an optimization problem, thus opening the door to colossal advances in data science methodologies. For instance, one of the methods developed is sparse identification of nonlinear dynamical systems (SINDy), which bridges differential equations and model development from data through sparse linear regression optimization problems to recover underlying equations from the data [36]. The connection between improved mathematical reasoning and big data optimization is fairly apparent when considering that improved modeling of different systems and better computational power can help with tasks relating to large datasets.

Furthermore, in finance, AI revolutionizes optimization techniques in algorithmic trading, risk management, and fraud detection by real-time analysis of vast databases, which in turn provides higher yields for algorithmic bases trading and reduces risk exposure [37]–[41]. These advancements could help both large and small firms stay afloat during market crashes, potentially stabilizing the economy as a whole. In fact, studies have proved that these machine learning systems could help reduce the heavy computational requirements affiliated with analyzing finances, leading to effective and efficient operations in the financial world [42].

In healthcare, particularly in medical research and diagnosis, advanced AI models capable of solving difficult mathematical issues can lead to improvements in predictive analytics [43]. These models are used to analyze complex data sets from medical records, imaging, and genomic data [44]–[47]. The potential contributions of AI in healthcare are highlighted by its proficiency in improving diagnostic accuracy and treatment plans [45], [46]. AI also finds applications in predictive analytics, supporting disease outbreak notification, resource planning, and personalized patient care [48]–[50].

In engineering, AI models optimize designing and manufacturing processes by churning the sensor data from production lines [51]. Through advanced mathematical models, AI can better process large volumes of data, therefore leading to improved optimization capabilities. The result of this can be visualized as improvements in product quality, efficiency, and preventive maintenance [51]. AI-driven big data optimization empowers engineers to make data-informed decisions, enhancing both operational performance and innovation [51].

The role of AI in environmental science and smart city planning cannot be overemphasized [52], [53]. AI models with this added adeptness can better analyze data from various sources for optimum parameters of planning, which may be—among other sectors—weather sensors, traffic systems, and energy grids, for urban planning and environmental monitoring [54]–[56]. This ensures the attainment of sustainable development and efficient resource allocation.

AI's potential contributions across many industries emphasize its relevance to sustainable AI—the development of artificial intelligence technologies in a way that reduces the carbon footprint and is economically, and socially responsible [57]. With better analytical abilities and more efficient data-churning processes, AI empowers sustainability. This is accomplished by cutting the time and expenses related to financial analysis, guaranteeing effective use of medical resources by aiding resource planning, and reducing waste by enhancing product quality. Furthermore, the development of sustainable cities depends on the processing speed of artificial intelligence models for analyzing data from traffic networks, electricity grids, etc. Good urban design could maximize the international resource economy, and raise the standard of living.

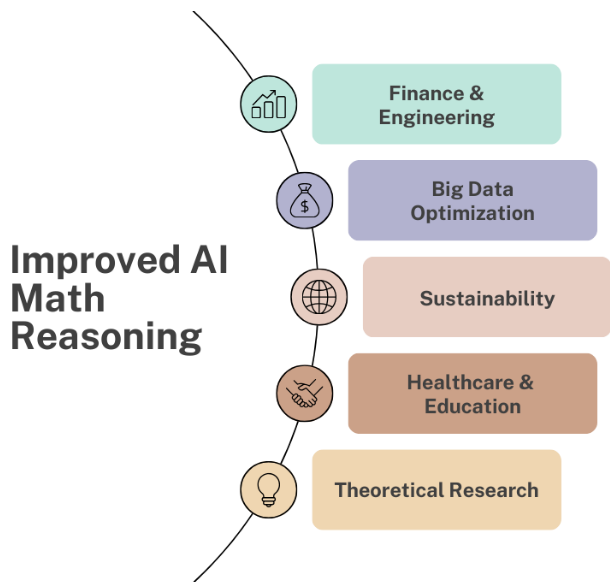

Fig. 4. Some of the various impacts of improved mathematical reasoning in artificial intelligence.

Although the aforementioned contributions of artificial intelligence are attributed to a more general improvement in the mathematical reasoning of AI models, various sustainability measures are directly advanced by solving differential equations. This is because the standard in sustainability revolves around simulating and forecasting the behavior of complex dynamic systems... exactly what differential equations are best utilized for. Neural ODEs, for instance, are a class of deep learning models that generalize their discrete-time counterparts utilizing differential equation integration into the learning process, which enables models to more successfully capture continuous and nonlinear dynamics [58], [59]. For sustainable uses like climate modeling and renewable energy management, precise forecasts generated by AI are more significant, hence this integration improves their capacity. This makes them strong for sustainability as it helps them to be practical under shifting climatic patterns or fluctuating energy sources.

V. Conclusion

This paper offers insightful analysis of six state-of-the-art artificial intelligence algorithms' ability to solve challenging mathematical problems—in particular complicated differential equations. This work opens the path for improved problem-solving abilities in many spheres, including education, healthcare, and theoretical research, by maximizing AI models for high-level mathematical reasoning.

Abbreviations

- **AI** - Artificial Intelligence
- **PINN** - Physics-Informed Neural Network
- **ML** - Machine Learning
- **LLM** - Large Language Model
- **PDE** - Partial Differential Equation
- **ODE** - Ordinary Differential Equation
- **SINDy** - Sparse Identification of Nonlinear Dynamical Systems
- **NLS** - Nonlinear Schrödinger Equation
- **NLP** - Natural Language Processing
- **DE** - Differential Equation
- **SDE** - Stochastic Differential Equation

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