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EVALUATING THE EFFECTIVENESS OF AI TOOLS IN MATHEMATICAL MODELLING OF VARIOUS LIFE PHENOMENA: A PROPOSED APPROACH

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ABSTRACT

Advances in artificial intelligence (AI) are transforming the landscape of mathematical modelling in areas including physics, biology, and chemistry. Research suggests that ChatGPT, Gemini, and other AI tools can change the way researchers use simulation and modeling for complex phenomena by helping to produce models faster with less computational complexity and real-time insights. Here, we introduce a novel framework for building mathematical models of life sciences using AI tools for applications in disease dynamics and ecological systems. The approach integrates AI tools into the process for a hybrid model that combines initial model formulations based on AI-assisted discussions and refinements based on expert validation of AI-generated output. To give an example, if we are interested in modelling disease outbreaks, AI platforms such as ChatGPT or Gemini can instantly build a simple susceptible-infectious-recovered (SIR) model. This also helps with high dataset processing and making parameter suggestions based on real-time data, which in turn helps in the dynamic adaptation of models to changing data (e.g. transmission rates or intervention strategies). Likewise, in ecological modelling, AI tools can aid in the generation of predator-prey models that consider these complex interactions, such as habitat fragmentation or reserved zones and then suggest parameter sensitivities based on observed trends. These abilities make the future of AI-based mathematical modelling especially exciting, as they will further decrease the time that is traditionally spent by researchers on manually defining models and allow them to focus on result interpretation and strategic decision-making. With the rapidly changing advances in AI tools, incorporating some new capabilities and developments in the mathematical modelling procedure may allow for unprecedented improvements in predictive performance, model flexibility and interdisciplinary investigations. Further research and real-world efforts with this approach are needed to determine if AI tools can improve the cost-effectiveness and affordability of mathematical modelling in many fields of science.

1. INTRODUCTION

Mathematical modelling [1] has historically represented an essential tool across many areas of research to gain insights into complex systems, from physics and biology to chemistry. Often based on foundational equations, these models provide researchers with the ability to simulate the behavior of natural phenomena. For example, in quantum mechanics, systems can be solved with the Schrödinger equation to facilitate predictions of particle behavior, thus leading to the advancement of technologies such as quantum computing and nanotechnology. In like manner, the Lotka-Volterra equations in ecology [2], [3] and the Hodgkin-Huxley model in computational

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biology [4] are models that succinctly express the fundamental dynamics of predator-prey dynamics and neuron dynamics, respectively. The examples highlight how mathematical models contribute to our scientific understanding of the world.

Although mathematical models are effective, they take a lot of time and expertise to construct and solve. This issue becomes increasingly severe as systems become more complex, as in the case of epidemiological models that use stochastic methods such as the Gillespie algorithm to model the transmission of disease in uncertain environments [5]. Additionally, with the availability of new data streams and data in which changes happen in real time, the necessity arises for models to track the changing environment adaptively. These issues create a demand for innovative methodologies that would simplify the model-building process while keeping or increasing the prediction performance.

Within this context, the evolution of artificial intelligence (AI) presents a promising opportunity for transforming mathematical modelling [6]-[10]. AI tools like ChatGPT, Gemini, and similar platforms have the potential to revolutionize how researchers build and refine models by automating certain aspects of model generation and reducing computational complexity. For example, AI-driven models can quickly adapt to new data inputs, suggesting adjustments to parameters in real-time. In the case of disease dynamics, platforms like ChatGPT and Gemini can assist in generating basic models, such as the susceptible-infectious-recovered (SIR) framework, and refine these models as transmission rates change or new interventions are introduced. Similarly, in ecological modelling, AI tools can facilitate the development of predator-prey models by incorporating complex variables such as habitat fragmentation or the effects of reserved zones.

Previous work on AI tools has demonstrated their utility across various disciplines. Within academic circles, ChatGPT, as one of these tools, has proven its relevance in fields ranging from education [11]-[14] and healthcare [15]-[21] to industry [22]-[29] and the creative arts [30],[31]. Studies have particularly noted its potential in mathematics education [32]-[45], where ChatGPT has been used to solve problems in linear algebra [46]-[49], word comprehension [50], and other mathematical domains [51]-[55]. However, there is a growing need to explore how these tools can be applied to more advanced mathematical modelling tasks, particularly in scientific research. Although AI models like ChatGPT have been extensively studied for their ability to solve isolated mathematical problems, their application to full-scale, dynamic mathematical modelling—such as those needed in disease dynamics or ecological systems—remains underexplored.

This paper addresses these gaps by proposing a framework for integrating AI tools like ChatGPT and Gemini into mathematical modelling workflows. Unlike previous studies that focus on isolated calculations, our approach leverages AI to generate initial models through interaction-based prompts, which are then refined with expert oversight. This allows for more adaptive, efficient, and accurate models that can evolve as new data becomes available. Our framework not only accelerates model development but also incorporates unstructured data sources, such as real-time observational data, into the modelling process—an area that has been largely unexplored in previous work.

The rest of this paper is organized as follows: In Section 1, we review the Research Background, discussing the mathematical equations in life phenomena modelling and the role of ai in computational mathematics. Section 2 presents the Problem Statement, identifying the key challenges and gaps in current approaches. Section 3 outlines the Research Objectives of our proposed framework, while Section 4 discusses the Scope and Limitations of the study. In Section 5, we highlight the Significance of the Research and its broader implications for the scientific community. Finally, Section 6 concludes with a summary of our contributions and directions for Future Research into the role of AI in mathematical modelling.

2. RESEARCH BACKGROUND

Mathematical modelling is a reasonable approach to understanding and determining numerous biological phenomena, which is commonly used across a variety of other fields of science. Additionally, formulating equations, as well as other computational techniques, can elucidate numerous complicated interactions that regulate all forms of life.

2.1 Mathematical Equations in Life Phenomena Modelling

Mathematical equations function as the medium by which we express the conduct and interplay of biological, chemical, and physical systems. These equations are further categorized into different types:

2.1.1 Ordinary Differential Equations (ODEs):

Ordinary Differential Equations are employed to illustrate dynamic systems of similar phenomena having only one independent variable (IV). For example, ODEs are applied in modelling population growth as well as disease spreading. It also has applications in dynamic-related chemistry problems on chemical reaction kinetics.

2.1.2 Partial Differential Equations (PDEs):

Partial Differential Equations further extend the complexity of ODEs by integrating multiple IVs. PDEs are deemed vital in modelling phenomena like heat conduction, fluid flow as well as the substances' diffusion.

2.1.3 Integro Differential Equations (IDEs):

Integro Differential Equations combine integral as well as differential equations. It integrates both instantaneous state information as well as accumulated history. This is valuable for concepts like viscoelastic material deformation or population dynamics over time.

2.1.4 Stochastic Processes:

Stochastic Processes are employed by numerous mathematical models in simulating systems that possess intrinsic randomness. These processes are valuable and are often employed in the application of risk handling, financial mathematics and specific areas of biology.

2.2 Role of AI in Computational Mathematics

AI has provided significant breakthroughs in computational mathematics. When it comes to identifying patterns, optimizing models, or solving complex equations, which are insurmountable for typical numerical techniques, AI algorithms have the ability to handle large data sets. One of the great strengths is that machine learning (ML), as a subfield of AI, utilizes data-driven methods in creating models that can improve both the precision and prognostic capacity of generalized mathematical simulations.

By providing researchers with explanations, coding generators, and insights, AI tools like ChatGPT and Gemini make the whole mathematical modelling process develop faster. As language models continue to improve in computational mathematics, it can be known that the field will move toward a larger role through their development into more sophisticated, nuanced, and expedited mathematical models.

3. PROBLEM STATEMENT

Despite improvements in mathematical modelling across a variety of scientific fields, the process of creating and testing models is complex, time-consuming, and computationally intensive. Mathematical models are fundamental in explaining and predicting the behavior of complex systems in physics, biology, chemistry, and beyond, utilizing equations to represent the intricate dynamics of natural phenomena. However, the traditional method for mathematical modelling remains time-consuming, not conducive to high-throughput computation and does not scale well with large-scale data size or near real-time consumption of data.

The advent of AI and specific advanced language models like ChatGPT and Gemini, which were created by OpenAI and Google, respectively, introduces a potential paradigm shift in how one does mathematical modelling. AI-driven tools offer helpful functionalities like generating human-like text, understanding context, and providing insights that could streamline the modelling process. However, the way in which ChatGPT, Gemini, and other proves to be effective and reliable for mathematical modelling assistance has not been largely explored. In particular, we seek insights into how AI tools can engage interactively with users to replicate the modelling process in different scientific contexts, computational precision, adaptability to a variety of data sets, and how reliably ChatGPT produces predictive modelling.

Based on the background outlined above, the primary problem proposed to be addressed by this study in the future is twofold: In particular, to assess how well AI tools can handle and further support the mathematical modelling process in relation to its computational accuracy, flexibility, and predictive reliability. Second, to determine the possible limitations and difficulties in incorporating AI-driven tools such as ChatGPT and Gemini into the mathematical modelling process. This study aims to perform a systematic evaluation of AI tools on mathematical modelling tasks, as well as benchmark its ability to improve the landscape in modelling complex phenomena seen in life and the universe.

4. RESEARCH OBJECTIVES

Mathematical modelling is, therefore, used to simulate and explain complex life phenomena in physics, biology, chemistry, etc., which is an interdisciplinary application. The advancements of AI have introduced a paradigm shift, with advanced algorithms enabling real-time data analysis and providing new-age insights.

This research aims to explore the ability of AI tools as mathematical modelling assistance. At the first level, we will go through some intentionally designed structured queries to simulate the modelling process of using ChatGPT across versatile contexts. The responses to these questions will be studied in detail and then benchmarked against well-established academic references to verify the abilities of our tool.

We aim to focus on the performance of AI tools like ChatGPT, Gemini, and other similar platforms from other aspects, including their computational accuracy, adaptability to variable data sets, as well as the reliability of their predictive modelling.

The results of this investigation aim to identify opportunities for and challenges faced by AI-driven tools in expanding possibilities within mathematical modelling with respect to our understanding of life and how its various phenomena. Hence, the research objectives will be identified as follows:

- To explore the potential of AI tools in enhancing the process of mathematical modelling for life phenomena: This objective focuses on investigating how AI tools like ChatGPT, Gemini, and other similar platforms can be integrated into the mathematical modelling process, examining their role in generating, refining, and improving models for various life phenomena such as Mathematical Epidemiology and Ecology.
- To assess the performance and reliability of AI-generated models in comparison to traditional methods: This objective aims to evaluate the models generated by AI tools like ChatGPT, Gemini, and other similar platforms by comparing their accuracy, efficiency, and robustness against traditional mathematical models and empirical data. The goal is to identify the strengths and limitations of using AI tools for mathematical modelling.

5. SCOPE AND LIMITATIONS

AI tools such as ChatGPT, Gemini, and other similar AI technologies build their models by training on a vast corpus of text data, including scientific literature, textbooks, educational resources, and other preparatory educational supplies until September 2021 [56]. It leverages a trained information framework for regular expertise and structural paradigms, although it does not draw on the latest information, resources or citations. In this work, we provide an initial exploration of how AI tools can inform mathematical modelling of life phenomena and of how its models compare to established models. This allows us to review how effective, accurate, and reliable the AI tool is. Although AI applications like ChatGPT, Gemini, and other subsequent tools prove to be an excellent start for initial models, researchers need to confirm and optimize these models. The scope and limitations of this study are outlined in this section as follows:

5.1 Scope of the Study

a. **Diverse Scientific Domains:** The research recommends adopting Artificial Intelligence (AI) tools, including ChatGPT, Gemini and other models in mathematical modelling in different domains, spanning computational biology, epidemiology, etc. This provides a complete review pertaining to the versatility of AI tools in enabling mathematical models, which vary between simple and complex depending upon different natures.

b. **Comparison with Established Models:** AI tools such as ChatGPT, Gemini, and other such platform proposals will have their performance subject to direct comparison with mathematical models that have been established in the scientific literature. Benchmarking is important for measuring the fidelity and reliability of AI-generated models.

c. **AI's Role in Mathematical Modelling:** The counternarratives proposed an improved mathematical modelling process wherein AI in the form of ChatGPT, Gemini and other platforms of a similar nature may play a more significant part. Its purpose is to highlight sites where the AI, with or against conventional modelling, can be employed, possibly making inaccessibly advanced mathematical tools available.

5-2 Limitations of the Study

a. **Scope of AI Interaction:** The interactions with AI tools like ChatGPT, Gemini, and other similar platforms are limited to structured queries within the boundaries of the model's training data and capabilities as of its last update. Thus, the performance of these tools on tasks or data beyond their training context could be different.

b. **Domain Expertise Requirement:** The interpretation and assessment of AI tools output requires a significant level of domain expertise. This requirement might make the results less generalizable to non-expert users and, hence, of broader applicability in mathematical modelling by AI.

c. **Evolution of AI Technology:** AI technology, such as language models like ChatGPT, Gemini, and others, is progressing rapidly. The outcomes and conclusions of this study may become less pertinent as the technology evolves through new, improved versions.

d. **Dependence on Benchmark Models:** The study proposed to compare AI tools like ChatGPT, Gemini, and other similar platforms to existing models based on the assumption that they are correct and complete. Since these are benchmark models, the performance of AI tools can be highly impacted by any deficiencies or inaccuracies in such baseline models.

6. SIGNIFICANCE OF RESEARCH

The significance of this research lies in its exploration of the integration of artificial intelligence, such as ChatGPT and Gemini, into the domain of mathematical modelling across various scientific disciplines. This study addresses a timely and critical inquiry into how AI-driven tools can enhance the traditional process of mathematical modelling, which is fundamental for understanding complex life phenomena in fields such as physics, biology, and chemistry.

6-1 Key Significance of the Research:

This research is important as the first study that proposes and investigates the utilization of artificial intelligence tools integration in mathematical modelling for many scientific areas. This research attempts to answer an important modern question on the role that AI-driven tools can play in improving a well-established process for mathematical modelling, essential for understanding complex life processes (or any other subject matter) by considering it from even broader areas like physics, biology, and chemistry.

a. **Innovative Integration of AI in Scientific Research:** It pioneers the evaluation of AI tools like ChatGPT, Gemini, and other similar platforms capacity to help in mathematical modelling, demonstrating that AI can enable new scientific understandings by simplifying the development of models and potentially changing the way scientific research is conducted.

b. **Enhancement of Mathematical Modelling Processes:** By assessing the effectiveness and computational accuracy of AI tools like ChatGPT, Gemini, and other similar platforms in assisting with mathematical models, this research will emphasize AI as an enabler for better efficiency, precision, and creativity in modelling complex systems.

c. **Bridging Computational and Empirical Analysis:** The study stands to bridge the gap between computational AI tools and empirical scientific approaches, offering a unique perspective on the synergy between computational intelligence and traditional scientific analysis.

d. **Expanding Accessibility to Complex Modelling:** By showing how AI tools like ChatGPT, Gemini, and other similar platforms may not only simplify but also expedite the modelling process, it has the potential to democratize access to sophisticated mathematical tools, making them more accessible to researchers and educators.

e. **Identifying Limitations and Setting Future Directions:** The findings will help provide a road map for future developments and improvements in AI-powered research methodologies by explicitly detailing the constraints or difficulties of incorporating AI into mathematical modelling.

7. CONCLUSION AND FUTURE WORK

A forward-looking perspective on the use of AI-driven tools, such as ChatGPT, Gemini and similar platforms, in the mathematical modelling process across scientific disciplines is outlined in this paper. The benefit appears obvious — AI could significantly improve the speed, accuracy, and flexibility of how we generate models even if (as far as I'm aware) this research hasn't been done yet. If leveraged, tools like ChatGPT and Gemini seem suitable to help quickly generate models that can be iteratively improved, particularly for complicated systems like disease dynamics and ecological interactions. AI could minimize the need for the time and expertise that traditional modelling tasks require by automating steps of the modelling process and making it easier to adapt directly to real-time data.

Our approach focuses on utilizing experts with maximum trust, experimentation, evaluation and cooperation with the AI-generated models. The current data handling and analysis methods will improve with the evolution of AI technology. Thus, its role in mathematical modelling will surely increase, creating possibilities for researchers to tap into AI skills for extending the range of mathematical modelling approaches, and thus improving the modelling precision.

This proposed approach, if implemented, could revolutionize the field by making sophisticated mathematical modelling more accessible and efficient. However, future research will be needed to fully validate the effectiveness and reliability of AI tools in this domain. The next steps should focus on exploring how AI can be refined for real-time model adaptation, managing complex datasets, and expanding its applicability across a wider range of scientific disciplines.

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CONFLICT OF INTEREST

The authors declare that there is *no conflict of interest* regarding the publication of this paper.

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