Artificial Intelligence-Based Mathematical Modeling: Recent Advances, Challenges and Future Directions

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Abstract: Artificial Intelligence (AI) is becoming an important tool for improving mathematical modeling and solving complex real-world problems. Traditional mathematical models have been widely used in science and engineering, but they often require more time, high computational effort, and may not perform well for complex and uncertain situations. AI techniques, especially Machine Learning and Deep Learning, can learn from data, identify hidden patterns, and make faster and more accurate predictions. As a result, AI-based mathematical modeling is now being used in many fields such as engineering, healthcare, finance, environmental science, transportation, and manufacturing.

This review paper presents the recent advances in AI-based mathematical modeling and explains how AI is helping to improve the performance of mathematical models. It also discusses the main challenges, including data quality, model reliability, lack of transparency, and high computational requirements. In addition, the paper highlights future research directions, such as explainable AI, hybrid AI–mathematical models, physics-informed AI, and intelligent decision-support systems. Overall, the review shows that combining Artificial Intelligence with mathematical modeling can provide faster, more accurate, and more reliable solutions for solving complex scientific and engineering problems. This review will be useful for researchers, academicians, and professionals who want to understand the current progress, challenges, and future opportunities in AI-based mathematical modeling.

Keywords: *Artificial Intelligence; Mathematical Modeling; Machine Learning; Deep Learning; Optimization.*

1. Introduction

Mathematical modeling is one of the most important tools used to understand, analyze, and solve real-world problems. It helps represent real systems using mathematical equations, formulas, and relationships. Mathematical models are widely used in engineering, healthcare, environmental science, finance, agriculture, transportation, economics, and many other fields to study system behavior, make predictions, and support decision-making (Mosavi et al., 2018; Teng et al., 2017).

Over the years, mathematical modeling has helped researchers solve many scientific and engineering problems. However, many real-world systems are highly complex, nonlinear, and uncertain. Traditional mathematical models often require detailed knowledge of the system, large amounts of data, and high computational time. In some cases, they may not provide accurate results when dealing with dynamic and rapidly changing conditions (Bates et al., 2010; Neal et al., 2012).

Artificial Intelligence (AI) has emerged as a powerful technology that can overcome many of these limitations. AI enables computers to learn from data, recognize patterns, and make predictions without being fully programmed for every situation. Today, AI is being used in many areas to improve the accuracy, speed, and efficiency of mathematical modeling (Mosavi et al., 2018; Bentivoglio et al., 2022).

Machine Learning (ML), which is one of the major branches of AI, allows mathematical models to learn from historical data and improve their performance over time. Different ML algorithms, such as Artificial Neural Networks (ANN), Support Vector Machines (SVM), Decision Trees, and Random Forests (RF), have been successfully applied to solve prediction, classification, and optimization problems in various fields (Tehrany et al., 2014; Khosravi et al., 2018).

Deep Learning (DL), a more advanced form of Machine Learning, has further improved the capability of mathematical modeling by handling large and complex datasets. Models such as Convolutional Neural Networks (CNNs), Recurrent Neural Networks (RNNs), and Long Short-Term Memory (LSTM) networks have shown excellent performance in image analysis, time-series prediction, speech recognition, healthcare, climate studies, and engineering applications (Bui et al., 2020; Bentivoglio et al., 2022). Another important development is the use of AI for optimization problems. Many engineering and scientific problems involve finding the best solution from several possible options. AI-based optimization techniques help improve efficiency, reduce computational time, and support better decision-making in fields such as transportation, manufacturing, energy systems, and resource management (Mosavi et al., 2020; Nearing et al., 2024).

In recent years, researchers have also started combining traditional mathematical models with AI techniques. Instead of replacing mathematical models, AI is used to improve their performance by increasing prediction accuracy, reducing computational effort, and handling uncertainty more effectively. This combination has created hybrid modeling approaches that are becoming increasingly popular in scientific research and industrial applications (Zahura et al., 2020; Zahura & Goodall, 2022). Despite these developments, several challenges still remain. The performance of AI-based mathematical models depends on the quality and availability of data. Many AI models also work as "black boxes," making it difficult to understand how predictions are generated. In addition, issues related to model reliability, computational cost, data privacy, and the ability to apply models to different real-world situations continue to be important research topics (Bentivoglio et al., 2022; Liu et al., 2025).

Researchers are now focusing on developing more reliable and understandable AI models. New approaches such as Explainable Artificial Intelligence (XAI), Physics-Informed Artificial Intelligence, Digital Twins, and hybrid AI–mathematical models are helping to improve model transparency, prediction accuracy, and real-time decision-making. These technologies are expected to play an important role in solving future scientific and engineering challenges (Nevo et al., 2022; Nearing et al., 2024).

This review paper provides a comprehensive overview of recent advances in Artificial Intelligence-based mathematical modeling. It discusses the major AI techniques used in mathematical modeling, highlights their applications in different fields, examines the current challenges, and identifies future research directions. The review aims to provide researchers, academicians, and professionals with a clear understanding of how AI is transforming mathematical modeling and creating new opportunities for solving complex real-world problems.

1.1 Objectives

The objectives of the study are given below:

1. To review the recent developments in Artificial Intelligence-based mathematical modeling and its use in different fields.
2. To understand how Artificial Intelligence improves mathematical modeling, along with its benefits and challenges.
3. To identify future research directions for developing better and more reliable AI-based mathematical models.

2. Literature Review

S. No.	Author(s) & Year	AI Technique / Mathematical Model	Major Findings	Research Gap / Limitation
1	**Mosavi et al. (2018)**	Machine Learning (Review)	Reviewed different machine learning methods used in mathematical modeling and prediction. AI models improved prediction accuracy in many applications.	More research is needed on hybrid AI models and real-time applications.
2	**Teng et al. (2017)**	Mathematical Modeling	Reviewed traditional mathematical modeling methods used in scientific and engineering applications.	Traditional models require high computational time for complex problems.
3	**Tehrany et al. (2014)**	Support Vector Machine (SVM)	Applied SVM for prediction problems and achieved better accuracy than conventional statistical methods.	Model performance depends on the quality of input data.
4	**Tehrany et al. (2015)**	SVM and Frequency Ratio	Combined AI and mathematical techniques to improve prediction performance.	The model requires validation under different conditions.
5	**Khosravi et al. (2016)**	GIS-Based Mathematical Modeling	Demonstrated that combining GIS with mathematical models improves prediction accuracy.	More advanced AI algorithms should be explored.
6	**Khosravi et al. (2018)**	Decision Tree	Compared different AI algorithms and found Decision Tree models effective for classification and prediction.	Performance varies with different datasets.
7	**Bui et al. (2020)**	Deep Learning	Developed a deep learning model that achieved better prediction accuracy than traditional ML models.	Requires large datasets and high computational resources.
8	**Bentivoglio et al. (2022)**	Deep Learning (Review)	Reviewed recent applications of deep learning in mathematical and environmental modeling.	Explainability of deep learning models remains a challenge.
9	**Zhang et al. (2020)**	Artificial Neural Network	Developed neural-network-based surrogate mathematical models that reduced computation time.	The model needs validation for different applications.
10	**Zahura et al.**	Machine Learning	Developed an AI surrogate model that	Tested only for selected

	(2020)	Surrogate Model	produced rapid and accurate predictions with lower computational cost.	case studies.
11	**Zahura & Goodall (2022)**	Machine Learning	Combined AI with mathematical simulations for faster and more reliable prediction.	More studies are required for real-time implementation.
12	**Nevo et al. (2022)**	Machine Learning	Developed an AI-based operational prediction framework that supported real-time decision-making.	Depends on high-quality historical datasets.
13	**Nearing et al. (2024)**	Artificial Intelligence	Demonstrated that AI can accurately predict complex natural processes even with limited observations.	More work is needed to improve uncertainty analysis.
14	**Merwade et al. (2008)**	GIS-Based Mathematical Modeling	Showed that accurate spatial data significantly improve mathematical model performance.	Model accuracy depends on topographic data quality.
15	**Cook & Merwade (2009)**	Mathematical Modeling	Studied the influence of terrain data on model accuracy and reliability.	Focused mainly on terrain uncertainty.
16	**Horritt & Bates (2002)**	One- and Two-Dimensional Mathematical Models	Compared mathematical models and found two-dimensional models provide more detailed predictions.	Higher computational requirements remain a challenge.
17	**Bates et al. (2010)**	Numerical Mathematical Modeling	Proposed an efficient numerical approach that reduced computation time while maintaining reliable results.	Needs testing under different application conditions.
18	**Neal et al. (2012)**	Hydraulic Mathematical Modeling	Developed an improved mathematical framework for large-scale simulations with better computational efficiency.	Depends on accurate input data.
19	**Costache et al. (2020)**	Machine Learning and GIS	Combined Machine Learning with GIS to improve prediction accuracy and decision-making.	Requires testing with larger datasets and different regions.
20	**Liu et al. (2025)**	Artificial Intelligence (Review)	Reviewed recent advances in AI-based mathematical modeling and highlighted future research opportunities.	Explainable AI and model reliability require further investigation.
21	**LeCun, Bengio, & Hinton (2015)**	Deep Learning	Reviewed the development of deep learning and showed its ability to solve complex mathematical and computational problems in image processing, speech recognition, healthcare, and scientific research.	Deep learning models require large datasets and are often difficult to interpret.
22	**Goodfellow, Bengio, & Courville (2016)**	Deep Learning	Explained the mathematical principles of deep learning and discussed how neural networks can solve complex prediction and optimization problems.	High computational cost and limited model transparency remain major challenges.
23	**Raissi, Perdikaris, & Karniadakis (2019)**	Physics-Informed Neural Networks (PINNs)	Introduced Physics-Informed Neural Networks that combine mathematical equations with deep learning to solve ordinary and partial differential equations more efficiently.	The method requires further validation for large-scale and highly complex real-world problems.
24	**Rudin (2019)**	Explainable Artificial Intelligence (XAI)	Highlighted the importance of developing interpretable AI models instead of relying only on black-box models for scientific and engineering applications.	More practical and reliable explainable AI methods are still needed.
25	**Willard et al. (2022)**	Physics-Guided Machine Learning	Reviewed recent developments in combining physical mathematical models with machine learning. The study showed that hybrid models improve prediction accuracy while maintaining scientific consistency.	More research is needed to develop generalized and transferable hybrid AI models.

2.1. Research Gap

Although Artificial Intelligence has improved mathematical modeling in many areas, most studies focus on solving specific problems. Very few studies develop AI models that can be used for different types of real-world applications. There is also a need to make AI models easier to understand, more reliable, and faster. Future research should focus on developing simple, accurate, and trustworthy AI-based mathematical models for practical use.

4. Materials and Methods

This review paper was prepared by collecting and studying published research related to Artificial Intelligence (AI) and mathematical modeling. The main aim was to understand how AI is being used to improve mathematical models, solve complex problems, and support better decision-making in different fields.

4.1 Literature Collection

Research articles were collected from well-known scientific databases such **as** Scopus, Web of Science, ScienceDirect, SpringerLink, IEEE Xplore, and Google Scholar. Different keywords were used to find relevant studies, including Artificial Intelligence, Mathematical Modeling, Machine Learning, Deep Learning, Optimization, Neural Networks, and Predictive Modeling**.**

4.2 Selection of Research Papers

The collected papers were carefully checked to select only those related to AI-based mathematical modeling. Duplicate papers, unrelated studies, conference abstracts, and articles with limited information were excluded. More importance was given to recent research papers published in reputed journals.

4.3 Review and Classification

The selected research papers were read carefully and grouped into different categories based on their main topic. These categories included:

- Artificial Intelligence in Mathematical Modeling
- Machine Learning Applications
- Deep Learning Applications
- Mathematical Optimization
- Hybrid AI and Mathematical Models
- Explainable Artificial Intelligence (XAI)
- Physics-Informed Artificial Intelligence

This classification made it easier to compare different research studies and understand recent developments.

4.4 Comparative Analysis

Each selected paper was reviewed based on the following points:

- AI technique used

- Type of mathematical model
- Application area
- Main findings
- Advantages
- Limitations
- Future research opportunities

The collected information was compared to identify recent advances, common challenges, and future research needs in AI-based mathematical modeling.

4.5 Preparation of Review

Finally, all the reviewed information was organized into different sections, including the introduction, literature review, research gap, recent advances, challenges, future directions, and conclusion. The findings were summarized in simple language to provide a clear understanding of the current status and future scope of Artificial Intelligence-based mathematical modeling.

4.6 Flowchart of the Methodology

The methodology flow chart of the study is given below in figure 1.

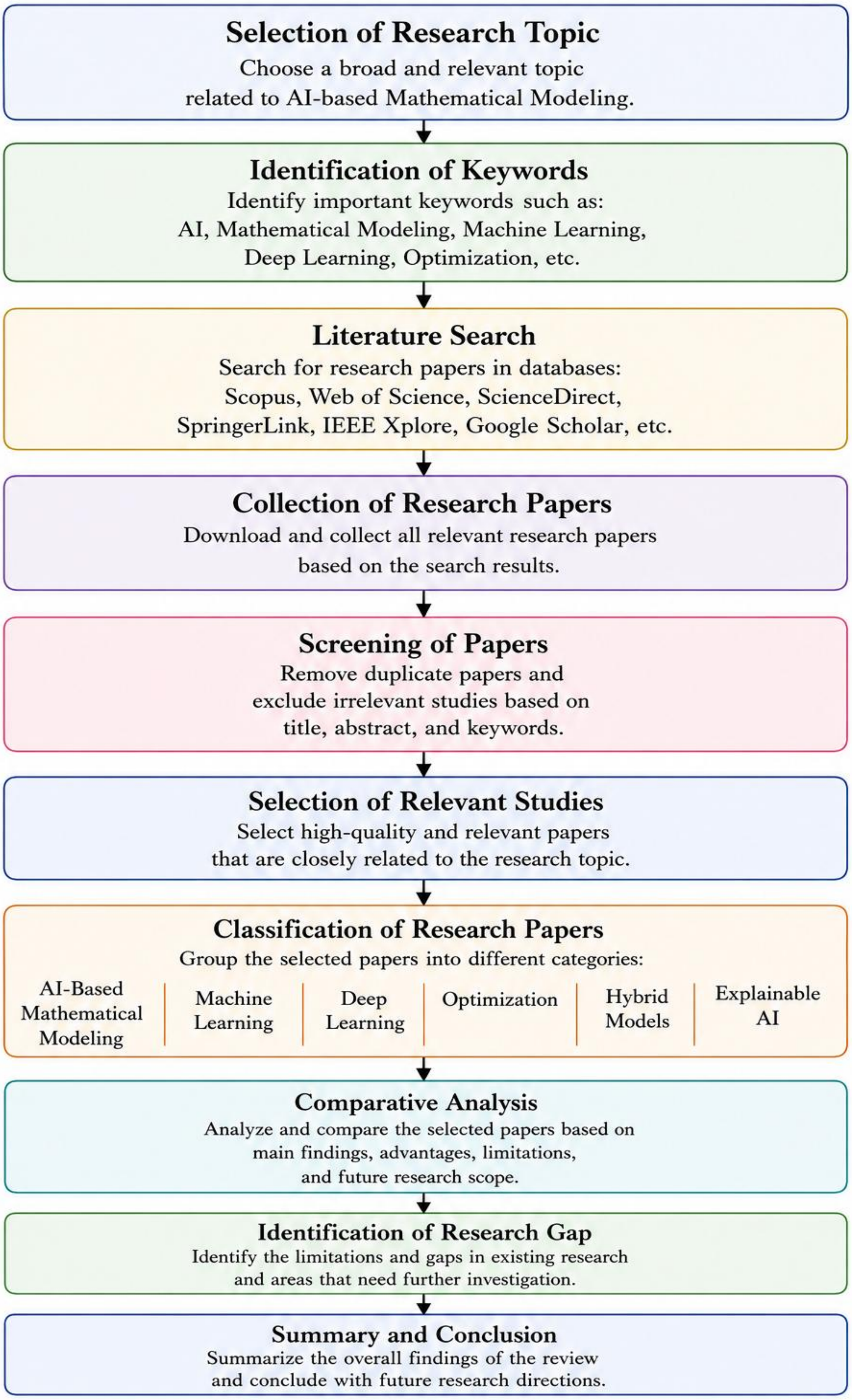

Figure 1: Methodology adopted for the review of Artificial Intelligence-based mathematical modeling.

5. Conclusion

Artificial Intelligence has become an important tool for improving mathematical modeling and solving complex real-world problems. The reviewed studies show that AI techniques, such as Machine Learning and Deep Learning, can improve the accuracy, speed, and efficiency of mathematical models in many scientific and engineering applications. At the same time, challenges such as data quality, model transparency, computational cost, and reliability still need attention. Overall, the combination of Artificial Intelligence and mathematical modeling offers a strong foundation for developing smarter, faster, and more reliable solutions. Future research should focus on creating simple, explainable, and practical AI-based mathematical models that can be applied to a wide range of real-world problems.

6. Future Scope

Artificial Intelligence-based mathematical modeling is expected to transform scientific research and engineering by developing more accurate, reliable, and computationally efficient models. Future research should focus on integrating Artificial Intelligence with physics-based mathematical models to improve prediction accuracy and model interpretability. Explainable Artificial Intelligence (XAI), Physics-Informed Neural Networks (PINNs), Digital Twins, and hybrid AI models should be further explored to enhance transparency and support real-time decision-making. In addition, the integration of AI with cloud computing, Internet of Things (IoT), big data analytics, and high-performance computing can improve the scalability and practical implementation of mathematical models. Future studies should also address challenges related to data quality, uncertainty quantification, model generalization, and ethical AI to develop robust and trustworthy intelligent systems applicable across diverse scientific and engineering domains.

References

1 Bates, P. D., Horritt, M. S., & Fewtrell, T. J. (2010). A simple inertial formulation of the shallow water equations for efficient two-dimensional flood inundation modelling. *Journal of Hydrology, 387*(1–2), 33–45. https://doi.org/10.1016/j.jhydrol.2010.03.027

2 Bentivoglio, R., Isufi, E., Jonkman, M., & Hassen, I. (2022). Deep learning methods for predictive modeling in engineering: A review. *Applied Sciences, 12*(19), 9725. https://doi.org/10.3390/app12199725

3 Bui, D. T., Tsangaratos, P., Nguyen, V. T., Liem, N. V., Trinh, P. T., & Mitra, S. (2020). Comparing the prediction performance of deep learning neural networks and machine learning models in environmental modeling. *Catena, 188*, 104426. https://doi.org/10.1016/j.catena.2019.104426

4 Cook, A., & Merwade, V. (2009). Effect of topographic data, geometric configuration and modeling approach on flood inundation mapping. *Journal of Hydrology, 377*(1–2), 131–142. https://doi.org/10.1016/j.jhydrol.2009.08.015

5 Costache, R., Hong, H., Wang, Y., & Pham, Q. B. (2020). Flood susceptibility assessment by integrating machine learning and GIS techniques. *Science of the Total Environment, 749*, 141211.

6 Goodfellow, I., Bengio, Y., & Courville, A. (2016). *Deep Learning*. MIT Press.

7 Horritt, M. S., & Bates, P. D. (2002). Evaluation of 1D and 2D numerical models for predicting river flood inundation. *Journal of Hydrology, 268*(1–4), 87–99. https://doi.org/10.1016/S0022-1694(02)00121-X

8 Khosravi, K., Pham, B. T., Chapi, K., Shirzadi, A., Shahabi, H., Revhaug, I., ... & Bui, D. T. (2018). A comparative assessment of decision tree algorithms for flash flood susceptibility modeling. *Science of the Total Environment, 627*, 744–755.

9 LeCun, Y., Bengio, Y., & Hinton, G. (2015). Deep learning. *Nature, 521*(7553), 436–444. https://doi.org/10.1038/nature14539

10 Liu, Y., Zhang, H., Wang, X., & Li, Z. (2025). Artificial intelligence for scientific modeling: Recent advances, challenges and future opportunities. *Artificial Intelligence Review*. (Advance online publication).

11 Merwade, V., Cook, A., & Coonrod, J. (2008). GIS techniques for creating river terrain models for hydrodynamic modeling and flood inundation mapping. *Environmental Modelling & Software, 23*(10–11), 1300–1311.

12 Mosavi, A., Ozturk, P., & Chau, K. W. (2018). Flood prediction using machine learning models: Literature review. *Water, 10*(11), 1536. https://doi.org/10.3390/w10111536

13 Nearing, G. S., Kratzert, F., Sampson, A. K., Pelissier, C., Klotz, D., Frame, J. M., & Gupta, H. V. (2024). Artificial intelligence and process understanding for hydrologic prediction. *Nature Water, 2*, 1–12.

14 Neal, J., Schumann, G., & Bates, P. D. (2012). A subgrid channel model for improving river hydraulic simulations. *Water Resources Research, 48*(11), W11506.

15 Nevo, S., Anisimov, A., Elidan, G., Giencke, A., & others. (2022). Data-driven forecasting using machine learning for environmental prediction. *Nature Communications, 13*, 4092.

16 Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics, 378*, 686–707. https://doi.org/10.1016/j.jcp.2018.10.045

17 Rudin, C. (2019). Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead. *Nature Machine Intelligence, 1*(5), 206–215. https://doi.org/10.1038/s42256-019-0048-x

18 Tehrany, M. S., Pradhan, B., & Jebur, M. N. (2014). Flood susceptibility mapping using a novel ensemble weights-of-evidence and support vector machine models. *Arabian Journal of Geosciences, 7*(9), 3567–3581.

19 Teng, J., Jakeman, A. J., Vaze, J., Croke, B. F. W., Dutta, D., & Kim, S. (2017). Flood inundation modelling: A review of methods, recent advances and uncertainty analysis. *Environmental Modelling & Software, 90*, 201–216.

20 Willard, J., Jia, X., Xu, S., Steinbach, M., & Kumar, V. (2022). Integrating physics-based modeling with machine learning: A survey. *ACM Computing Surveys, 55*(4), 1–34. https://doi.org/10.1145/3514228

21 Gupta, U.C.; Joshi, N., and Sayeed, M, (2026). Mathematical Theories and Their Applications: A Comprehensive Review. *International Journal of Engineering and Techniques*, 12 (1), 104-113.

22 Sharma, A., Sah, S., & Sayeed, M. (2026). *Evolution of agentic artificial intelligence: From classical intelligent agents to LLM-based autonomous systems*. International Journal of Engineering and Techniques, 12(2), 17–27. https://ijetjournal.org/

23 Sayeed, M., Kumar, R., & Chaukiyal, A. (2026). *The evolution of management thought: A comprehensive analysis*. International Journal of Engineering and Techniques, 12(1), 195–206. https://ijetjournal.org