

Advances in Applications of Artificial Intelligence for Predictive Modeling in Applied Sciences

Shiv Kumar ^{1*}

¹Department Of CSE, Galgotias University , Uttar Pradesh 203201 , India

*Corresponding Authors Email: shivkcse729@gmail.com

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Abstract: Recent advances in artificial intelligence (AI) have significantly transformed predictive modeling across a wide spectrum of applied sciences. This review explores the integration of AI techniques such as machine learning, deep learning, and hybrid models into predictive frameworks within disciplines including environmental science, engineering, healthcare, and materials science. These methods have demonstrated superior capabilities in handling complex, nonlinear, and high-dimensional data, enabling more accurate forecasts and decision-making tools. The paper highlights key developments in AI-driven algorithms, including neural networks, ensemble models, and reinforcement learning, while also examining their application in real-world scenarios like climate modeling, disease prediction, and structural integrity analysis. Emphasis is placed on the shift from traditional statistical approaches to data-driven methodologies that leverage big data and real-time analytics. Additionally, the review addresses current challenges such as model interpretability, data quality, and computational costs, and outlines future research directions focused on explainable AI, model generalization, and interdisciplinary integration. Overall, this paper provides a comprehensive overview of how AI is revolutionizing predictive modeling in applied sciences, fostering innovations that are shaping the future of scientific discovery and technological advancement.

Keywords : Artificial Intelligence, Predictive Modeling, Machine Learning, Applied Sciences, Data-Driven Methods

1. Introduction

Artificial Intelligence (AI) has become a cornerstone technology in the modern era, driving innovations across industries and transforming how scientists and engineers approach predictive modeling.[1] Predictive modeling, which relies on historical and real-time data to forecast future outcomes, is essential for applied sciences such as healthcare, civil engineering, environmental studies, materials science, and industrial processes. Traditionally, predictive modeling relied heavily on statistical methods and mechanistic models that, while useful, were often limited by their inability to process large volumes of data and account for complex nonlinear relationships. AI has addressed these limitations by enabling systems that can learn from data, adapt to new information, and provide accurate forecasts even in uncertain conditions. In applied sciences, AI algorithms enhance the ability to interpret multidimensional data from diverse sources, including sensors, simulations, and experimental results. For instance, in climate science, AI improves the accuracy of models predicting global warming and extreme weather events, while in healthcare, machine learning models outperform traditional risk scoring methods by identifying subtle patterns in patient data that predict disease progression. In industrial operations, AI facilitates predictive maintenance, ensuring that machines are serviced before they fail, thus reducing downtime and costs. The breadth of AI applications demonstrates its ability to bridge the gap between theoretical modeling and real-world deployment.[2] The significance of AI in predictive modeling extends beyond accuracy; it also enhances scalability, adaptability, and interpretability. AI systems can integrate heterogeneous data sources, from satellite imagery to medical records, enabling more comprehensive and context-aware predictions. Furthermore, AI can automate repetitive tasks, freeing researchers to focus on innovation and hypothesis testing. Recent developments in explainable AI have also addressed concerns about the “black-box” nature of machine learning models, increasing their acceptance in policy-driven fields. The growing interest in AI-driven predictive modeling is evident in the surge of publications, investments, and real-world deployments across applied

sciences. This surge is fueled by advances in computing power, the availability of big data, and breakthroughs in algorithmic research.[3] However, despite these advancements, challenges remain, including data quality issues, computational constraints, and ethical considerations regarding fairness and bias. To fully harness the potential of AI in predictive modeling, it is crucial to understand the current state of the field, its technological foundations, its diverse applications, and the future research directions that can address existing limitations. This review explores the evolution and current state of AI in predictive modeling for applied sciences. It begins by outlining the scope and objectives of the analysis, then delves into key technologies and methods that underpin recent innovations. A comparative analysis of AI applications in climate and urban system modeling is provided to highlight domain-specific strategies and challenges. The review also discusses recent trends, breakthroughs, and limitations before concluding with future directions and a summary that underscores the transformative impact of AI in this critical area of research.[Fig. 1]

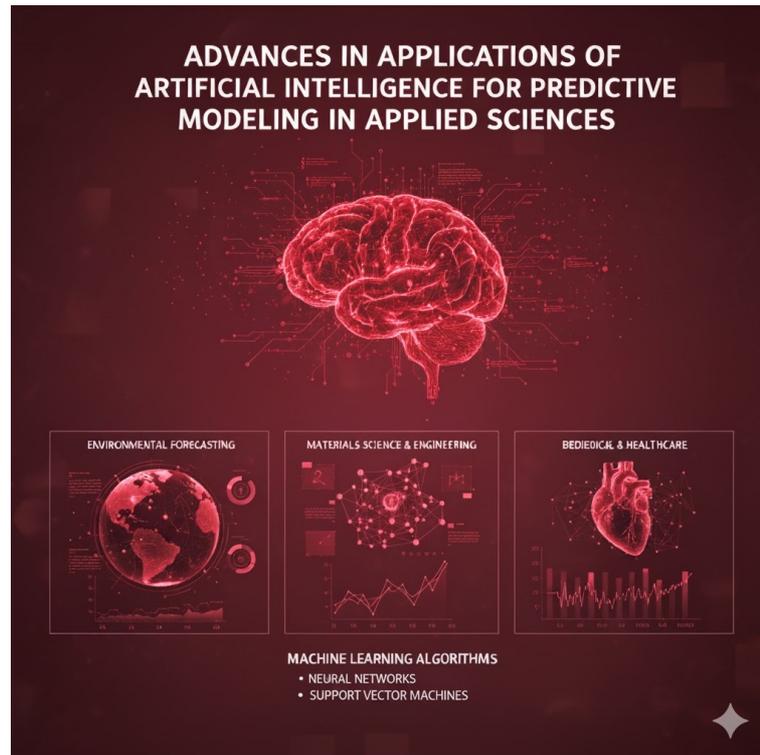


Fig. 1 Artificial intelligence for predictive modelling

2. Scope and Objectives of the Review

The scope of this review is to examine the role of Artificial Intelligence in predictive modeling within the context of applied sciences, encompassing a wide range of domains such as environmental science, healthcare, urban systems, industrial engineering, and materials science. AI's transformative potential lies in its ability to process complex data, generate accurate predictions, and enhance decision-making processes. This review covers both traditional AI methods like machine learning and advanced techniques such as deep learning, physics-informed neural networks, and agentic AI systems.[4] The objectives of the review are multifaceted. First, it aims to provide a comprehensive understanding of the technologies and methods that enable AI's predictive capabilities in applied sciences. By focusing on the technological underpinnings, this review highlights how algorithms have evolved from simple linear models to complex architectures capable of handling high-dimensional, heterogeneous data. Second, the review seeks to analyze how AI applications differ across domains by presenting a comparative analysis of climate modeling and urban system modeling, two areas where predictive accuracy is crucial for policy and operational decisions. This comparison reveals shared challenges, distinct methodologies, and unique priorities. Additionally, the review aims to identify and discuss recent trends and advancements that have propelled AI forward, including the integration of physics-informed learning, real-

time IoT-driven predictions, and explainability.[5] Another key objective is to examine the limitations and challenges that hinder broader adoption, such as ethical concerns, data privacy issues, and the computational demands of advanced models. Finally, this review aims to project future research directions, suggesting how the field can evolve through hybrid models, interdisciplinary collaboration, and sustainable AI practices. By achieving these objectives, the review provides a clear roadmap of the current landscape and future potential of AI in predictive modeling for applied sciences.

3. Key Technologies and Methods

The foundation of AI's success in predictive modeling lies in its diverse set of technologies and methods, each tailored to address specific challenges and data characteristics in applied sciences.[6] Machine learning algorithms, including Random Forests, Gradient Boosting Machines, and Support Vector Machines, are widely employed due to their ability to capture complex relationships in data without explicit programming. Random Forests, for example, aggregate predictions from multiple decision trees to improve accuracy and reduce overfitting, making them effective in predicting disease outcomes and assessing structural risks in civil engineering. Gradient Boosting algorithms build models sequentially, correcting errors from previous iterations, and are extensively used in energy consumption forecasting and risk assessment models[9]. Deep learning represents a significant leap forward, enabling AI to process unstructured and high-dimensional data. Convolutional Neural Networks (CNNs) excel in image-based predictions, such as analyzing satellite imagery for environmental monitoring or detecting anomalies in medical scans.[7] Recurrent Neural Networks (RNNs), particularly Long Short-Term Memory (LSTM) networks, are adept at handling sequential data, making them valuable in predicting traffic flows, stock prices, and patient health trajectories. Graph Neural Networks (GNNs) have emerged as powerful tools for analyzing relational data, particularly in urban networks and molecular structures, offering new possibilities for predictive modeling in transportation systems and drug discovery [11]. Physics-Informed Neural Networks (PINNs) bridge the gap between data-driven learning and scientific knowledge by embedding physical laws into the learning process. This integration ensures that predictions respect conservation laws and other domain-specific constraints, which is crucial for fields like fluid dynamics, climate science, and structural analysis. PINNs have been successfully applied in modeling groundwater flow, heat transfer, and atmospheric dynamics, demonstrating higher reliability than purely data-driven models [8]. Similarly, hybrid models that combine machine learning with optimization algorithms, such as Particle Swarm Optimization (PSO) or Genetic Algorithms (GA), enhance prediction accuracy in complex engineering problems. Agentic AI systems represent another breakthrough, as they can autonomously plan, reason, and conduct experiments. Unlike traditional AI, which depends on predefined datasets, agentic systems iteratively generate hypotheses, design experiments, and analyze results, accelerating scientific discovery in chemistry, materials science, and biology [2]. These systems have already demonstrated success in automating the design of catalysts, optimizing biological pathways, and discovering new materials with desirable properties. The integration of AI with the Internet of Things (IoT) and edge computing has opened new avenues for real-time predictive modeling. IoT networks provide continuous streams of data from sensors embedded in infrastructure, vehicles, and industrial machines, enabling AI models to make timely predictions and trigger automated responses. Edge computing ensures that data is processed close to its source, reducing latency and enhancing responsiveness, which is particularly valuable in applications such as autonomous driving and industrial safety monitoring. Explainable AI (XAI) has become increasingly important as complex AI models are deployed in sensitive domains where transparency is essential. Techniques such as SHAP (SHapley Additive exPlanations) and LIME (Local Interpretable Model-agnostic Explanations) allow stakeholders to understand how models arrive at predictions, fostering trust and accountability. In healthcare, for instance, XAI helps clinicians interpret AI-driven diagnostic suggestions, while in climate science, it aids policymakers in understanding the factors influencing predictive outcomes (BMJ, 2024). Federated learning addresses data privacy concerns by allowing AI models to learn from distributed data without centralizing sensitive information, a significant advancement for healthcare and finance. Overall, the diversity of AI technologies—from traditional ML to advanced deep

learning and agentic systems—provides applied sciences with a rich toolkit for predictive modeling. Each method offers unique advantages, and ongoing research focuses on combining them into hybrid frameworks that maximize accuracy, efficiency, and interpretability across various domains.

4. Comparative Analysis of Literature

The application of AI in predictive modeling can be illustrated through a comparison of climate modeling and urban system modeling, two domains that rely heavily on accurate forecasts for decision-making. Climate modeling traditionally depends on physics-based simulations, which, while comprehensive, require significant computational resources and often struggle with uncertainties arising from incomplete data. AI has enhanced these models by assimilating large volumes of observational and simulation data, improving predictions of extreme weather events, global warming impacts, and ecosystem changes [10]. Machine learning models, including ensemble methods and hybrid neural networks, have been used to correct biases in traditional climate models, making forecasts more reliable and actionable. In contrast, urban system modeling focuses on real-time optimization and operational management, where predictive accuracy must be achieved within tight time constraints. AI models in this domain leverage data from IoT sensors, traffic cameras, and social media to optimize traffic flow, energy consumption, and emergency response strategies. Physics-informed approaches combined with deep learning have been employed to enhance infrastructure resilience and reduce congestion. Unlike climate models, urban predictive systems prioritize immediacy and scalability, often using lightweight algorithms that can run on edge devices [7]. The strengths and limitations of AI in these domains reflect their distinct priorities. Climate modeling benefits from hybrid models that integrate scientific knowledge, but it faces ethical concerns regarding fairness and equity in policy decisions based on AI forecasts. Urban models enjoy rich data streams and strong predictive performance, but their computational demands can be prohibitive when scaled to large cities. Both domains share a reliance on hybrid AI techniques that combine domain knowledge with data-driven insights, and both require interdisciplinary collaboration to ensure predictions are accurate, interpretable, and socially responsible. This comparative analysis highlights how AI adapts to the unique needs of different applied sciences. While climate modeling leverages AI to enhance long-term predictions under uncertainty, urban systems use it to make real-time decisions with immediate impact. The comparison underscores the importance of tailoring AI methods to domain-specific challenges and integrating ethical considerations to ensure responsible use.

5. Recent Trends and Advancements

Recent years have witnessed remarkable trends and advancements in the application of AI for predictive modeling. One major trend is the widespread adoption of physics-informed AI, which combines the strengths of data-driven learning with domain-specific scientific principles. This approach has proven effective in environmental and civil engineering applications, where predictions must adhere to physical laws while compensating for data limitations [11]. Another significant development is the rise of agentic AI, which enables autonomous scientific discovery by automating hypothesis testing and experimental workflows. These systems have accelerated research in materials science and synthetic biology, leading to faster identification of optimal compounds and biological pathways [10]. In healthcare, AI has advanced to a level where it can predict disease progression with greater accuracy than traditional methods. Models for Alzheimer's disease and Acute Respiratory Distress Syndrome (ARDS) have demonstrated superior predictive power, enabling earlier interventions and improved patient outcomes [8]. Industrial operations have also been transformed by predictive maintenance powered by AI, which forecasts equipment failures before they occur, minimizing downtime and optimizing resource allocation (ResearchGate, 2025). These advancements have been complemented by explainable AI techniques that increase transparency and trust among stakeholders. Synthetic biology has embraced AI to design genetic circuits, optimize metabolic pathways, and enhance CRISPR efficiency. AI-driven models have also facilitated protein folding predictions, accelerating drug discovery and biotechnological innovations (PubMed, 2025). In climate science, AI models have improved the prediction of extreme events such as floods, droughts, and wildfires by addressing data scarcity through hybrid approaches that combine

observational data with simulation outputs (Nature Communications, 2025). Across all domains, the integration of AI with IoT and edge computing has enabled real-time monitoring and predictions, enhancing responsiveness and operational efficiency. These advancements indicate that AI is not merely a tool but a driving force behind scientific and technological progress. The ability to combine multiple data sources, learn complex patterns, and integrate domain knowledge positions AI as a transformative element in predictive modeling. However, these trends also highlight the need for responsible deployment, as the growing reliance on AI raises questions about transparency, fairness, and sustainability.

6. Future Directions

The future of AI in predictive modeling for applied sciences promises even greater advancements, driven by several key research directions. One critical area is the development of scalable hybrid architectures that combine the interpretability of physics-informed models with the flexibility of deep learning. Such architectures can bridge the gap between scientific understanding and data-driven predictions, ensuring that models are both accurate and trustworthy. Agentic AI is expected to play a larger role in automating scientific discovery. These autonomous systems will not only analyze data but also design and execute experiments, significantly accelerating innovation in chemistry, biology, and materials science [2]. To build trust and facilitate adoption, future AI models must also prioritize explainability and fairness. Incorporating ethical frameworks and fairness-aware algorithms will be essential to prevent biases and ensure that predictions do not disproportionately impact vulnerable populations. Another promising direction is the democratization of AI through tools like Automated Machine Learning (AutoML), which simplifies model development, and edge computing, which enables low-latency predictions even in resource-constrained environments. Federated learning will further expand AI's reach by allowing models to learn from distributed data while preserving privacy, a critical factor in healthcare and finance. Sustainability will also become a major focus, as large AI models consume substantial energy. Researchers are exploring energy-efficient architectures and green AI practices to minimize environmental impact. Moreover, interdisciplinary collaboration will be crucial for the future of AI in applied sciences. Bringing together AI specialists, domain experts, policymakers, and ethicists will ensure that predictive models are contextually relevant, ethically sound, and aligned with societal needs. Ultimately, the future lies in creating AI systems that are not only powerful but also interpretable, fair, and sustainable. These systems will drive breakthroughs across applied sciences, enabling more accurate predictions, faster discoveries, and better-informed decisions.

7. Summary

Artificial Intelligence has revolutionized predictive modeling across applied sciences, enhancing the accuracy, scalability, and interpretability of forecasts in domains ranging from healthcare to climate science. By leveraging technologies such as machine learning, deep learning, physics-informed neural networks, and agentic AI, researchers have developed models capable of processing complex, multidimensional data and generating actionable insights. The integration of AI with IoT, edge computing, and explainable frameworks has further expanded its applicability, enabling real-time predictions and increasing stakeholder trust. A comparison between AI applications in climate modeling and urban systems reveals how domain-specific challenges shape methodological choices. Climate models emphasize long-term predictions under uncertainty, relying on hybrid approaches that combine physical knowledge with data-driven learning. Urban models, in contrast, prioritize real-time optimization, leveraging dense sensor data and lightweight algorithms. Both domains benefit from interdisciplinary collaboration and hybrid AI techniques that enhance predictive reliability. Recent trends, including the rise of physics-informed AI, agentic AI, and explainable frameworks, have propelled the field forward. Advances in healthcare, synthetic biology, industrial maintenance, and climate prediction demonstrate the versatility of AI-driven approaches. However, challenges such as data quality issues, computational demands, and ethical concerns must be addressed to ensure responsible deployment. Looking ahead, future research should focus on scalable hybrid models, autonomous agentic systems, fairness-aware algorithms, and sustainable AI practices. Interdisciplinary collaboration will play a vital role in aligning AI innovations with societal goals. As

these advancements unfold, AI is poised to become an indispensable tool in predictive modeling, driving discoveries and shaping decision-making in applied sciences.

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