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Integrating AI Techniques into Mathematical Modelling of Complex Systems

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Abstract- Mathematical modelling is a cornerstone of understanding and predicting complex systems in fields ranging from physics and biology to economics and engineering. With the advent of Artificial Intelligence (AI), especially machine learning and deep learning techniques, there has been a transformative shift in how models are constructed, validated, and interpreted. This paper explores the integration of AI into mathematical modelling, discussing the synergies between traditional analytical methods and modern computational intelligence. Case studies in epidemiology, climate modelling, and financial forecasting are reviewed to illustrate the practical applications and benefits of this integration. Challenges and future research directions are also discussed.

Keywords- Mathematical Modelling, Artificial Intelligence (AI), Machine Learning, Deep Learning, Computational Intelligence, Hybrid Modelling, Data-Driven Models, Model Integration

I. INTRODUCTION

Mathematical modelling involves the abstraction and representation of real-world systems through mathematical expressions and equations. Traditional modelling relies on domain knowledge and analytical tools to build models that are both interpretable and predictive. However, many real-world systems exhibit nonlinear, high-dimensional, and stochastic behaviours that challenge conventional approaches. AI, particularly data-driven models, has emerged as a powerful complement to traditional mathematical modelling.

II. ROLE OF AI IN MATHEMATICAL MODELLING

AI techniques, particularly machine learning (ML) and deep learning (DL), can handle large datasets, detect complex patterns, and approximate unknown functions without explicit programming. These capabilities make them ideal for:

- **Model construction**: AI can suggest model structures or directly learn models from data.
- **Parameter estimation**: AI methods can optimize parameters in ways traditional techniques may struggle with.
- **Model validation and refinement**: AI can automate validation processes and adapt models dynamically as new data becomes available.

III. CASE STUDIES EPIDEMIOLOGICAL MODELLING

In the context of infectious disease modelling, AI has been used to forecast outbreaks, estimate transmission rates, and simulate intervention strategies.

For example, machine learning models have been employed alongside SIR-type compartmental models to improve prediction accuracy (Yang et al., 2020).

A suitable example of such integration is the AI-enhanced SEIR (Susceptible-ExposedInfectious-Recovered) model, where deep learning is used to dynamically estimate parameters like transmission and recovery rates. In this hybrid approach, the classical SEIR model provides the mechanistic framework, while neural networks—particularly recurrent neural networks (RNNs) or long short-term memory networks (LSTMs)—learn timedependent parameters from real-time data. This improves the adaptability and predictive accuracy of the model during rapidly evolving situations such as a pandemic. For instance, the transmission rate β(t) can be learned from daily case reports using an LSTM network, which captures temporal patterns and lagged effects. Such models are particularly valuable for simulating the impact of public health interventions, as they can adjust forecasts based on current policy or mobility data. This synergy between AI and classical modelling enhances both interpretability and responsiveness, making it a powerful tool for decision-makers during public health crises. In the context of infectious disease modelling, AI has been used to forecast outbreaks, estimate transmission rates, and simulate intervention strategies. For example, machine learning models have been employed alongside SIR-type compartmental models to improve prediction accuracy (Yang et al., 2020).

AI-Enhanced SEIR Model: Mathematical Formulation

The classical SEIR model is defined by the following system of differential equations:

$$\frac{dS}{dt} = -\beta(t).\frac{S(t).I(t)}{N}$$

$$\frac{dE}{dt} = \beta(t).\frac{S(t).I(t)}{N} - \sigma E(t)$$

$$\frac{dI}{dt} = \sigma E(t) - \gamma I(t)$$

$$\frac{dR}{dt} = \gamma I(t)$$

Where:S(t), E(t), I(t), R(t) are the susceptible, exposed, infectious, and recovered populations at time t, N is the total population, β(t) is the time-varying transmission rate (learned via AI), σ is the rate at which exposed individuals become infectious, γ is the recovery rate.

In the AI-enhanced version, the function β(t)\beta(t)β(t) is modeled using a Long Short-Term Memory (LSTM) network, trained on daily infection data, mobility reports, and public policy indicators. The learned β(t) captures temporal dynamics and external influences that are hard to model analytically.

This hybrid approach combines the interpretability and epidemiological grounding of compartmental models with the adaptive learning capabilities of AI, providing more accurate and flexible forecasts in real-time outbreak scenarios.

III. CLIMATE MODELLING

AI has contributed to enhancing the spatial and temporal resolution of climate models through super-resolution techniques and emulation of sub-grid processes.

DL models have been trained on climate simulation outputs to provide faster and more detailed forecasts (Reichstein et al., 2019).

A concrete example is the use of convolutional neural networks (CNNs) for downscaling coarse-resolution climate model outputs. These super-resolution models learn mappings from low-resolution inputs—such as those generated by general circulation models (GCMs)—to high-resolution climate patterns. For instance, Vandal et al. (2017) applied CNN-based architectures to improve precipitation estimates at a finer spatial scale, achieving more accurate regional climate predictions. Additionally, AI models have been employed to emulate computationally intensive components of Earth system models. By replacing physics-based components with trained neural networks, researchers have reduced simulation runtimes significantly while preserving fidelity. Such emulation techniques are particularly effective for long-term climate projections and sensitivity analyses. These advancements allow scientists and policymakers to better understand localized climate risks and design targeted adaptation strategies.

Model Example: Super-Resolution Convolutional Neural Network (SRCNN)

The Super-Resolution Convolutional Neural Network (SRCNN) is a pioneering deep learning model initially developed for image super-resolution, but it has been effectively adapted for climate downscaling — enhancing the spatial resolution of coarse climate model outputs.

Basic Architecture of SRCNN

SRCNN consists of three main convolutional layers, each performing a specific role in the transformation from low-resolution (LR) to high-resolution (HR) data:

Patch Extraction and Representation:

- A convolutional layer extracts overlapping patches from the low-resolution input climate data.
- These patches are projected into a high-dimensional feature space.

Mathematically:

$F1(Y) = \max(0, W1 * Y + B1)$

where Y is the LR input, W1 are learned filters, and B1 is the bias.

Non-linear Mapping:

- This layer maps the extracted LR feature representations into HR feature space using a non-linear transformation.

Mathematically:

$F2 = \max(0, W2 * F1 + B2)$

Reconstruction Layer

The final layer aggregates the high-resolution features to reconstruct the final

HR output.

Mathematically:

$\hat{X} = W3 * F2 + B3$

Where:

* denotes the convolution operation,

W1, W2, W3 and B1,B2,B3 are the learnable weights and biases, ReLU (Rectified Linear Unit) is commonly used as the activation function.

Application in Climate Downscaling

- SRCNN models have been successfully applied to enhance resolution in various climate
- variables, such as: Surface temperature, Precipitation, Wind fields etc.
- These models can generate high-resolution outputs that closely match the fidelity of
- traditional dynamical downscaling approaches, but with significantly lower computational costs.

Advantages of SRCNN in Climate Science

- Efficient training and inference
- Flexible architecture adaptable to multi-channel climate data
- High accuracy in capturing spatial variability
- Scalable to global or regional datasetsSRCNN models have been successfully applied to improve resolution in temperature and precipitation data, yielding outputs comparable to high-resolution simulations but at a fraction of the computational cost. (Vandal et al., 2017) (Reichstein et al., 2019)

IV. FINANCIAL FORECASTING

In finance, AI has improved the modelling of stock prices and risk assessment. Hybrid models combining econometric techniques with neural networks have demonstrated improved predictive power (Fischer & Krauss, 2018).

A notable example is the use of Long Short-Term Memory (LSTM) networks for predicting stock market trends based on both historical prices and sentiment analysis from news headlines. In the study by Akita et al. (2016), LSTM models were trained on time-series data of stock prices along with textual sentiment extracted from financial news using natural language processing (NLP). The integration of qualitative sentiment data allowed the model to better anticipate market reactions to events and news releases. This approach demonstrated higher prediction accuracy compared to models relying solely on quantitative data. Such

AI driven models are valuable tools for traders and financial analysts seeking to gain a competitive edge in volatile markets, and they underscore the potential of combining deep learning with alternative data sources for financial forecasting.

LSTM Based Sentiment Enhanced Financial Forecasting

Model Example: LSTM-Based Sentiment-Enhanced Financial Forecasting The LSTM-based financial forecasting model consists of two main input streams:

Historical Price Data: Used as a time-series input to model price trends and volatility
patterns.

Sentiment Scores: Extracted from financial news articles and social media using NLP techniques such as sentiment analysis and word embeddings.

These inputs are concatenated and passed into an LSTM network, which captures long-term dependencies in sequential data. The final dense layer outputs the predicted stock price or return.

Mathematically, the model predicts the price Pt+1
Pi+1 at time t + 1 based on previous prices
Pi-n,..., Pi and sentiment Si .
Pi+1 = fLSTM([Pi - n. .., Pi], St)
Where:
fLSTM is the learned LSTM function,

St is the aggregated sentiment score at time t. This architecture allows the model to not only learn temporal price trends but also incorporate contextual market sentiment, resulting in more responsive and informed predictions.

(Akita et al., 2016)

V. CHALLENGES AND LIMITATIONS

Despite their potential, AI models are often criticized for their lack of interpretability, overfitting risks, and dependency on large, high-quality datasets. Integrating domain knowledge into AI models and developing hybrid models that retain mathematical interpretability are ongoing research areas.

Lack of Interpretability

AI models, particularly deep neural networks, are often referred to as **"black boxes"** because:
It's hard to understand *how* and *why* they make certain decisions.

This poses problems in critical domains like healthcare, finance, and law, where **transparency** and **explainability** are essential.

Explainable AI (XAI) is an emerging field trying to tackle this through methods like:

- Feature importance techniques (e.g., SHAP, LIME)
- Model distillation
- Attention mechanisms

Overfitting Risks

Overfitting happens when models **memorize** training data instead of learning general patterns.
This leads to poor generalization on unseen data.
Causes include:

- Small or noisy datasets
- Excessive model complexity
- Common solutions:
- Regularization techniques (L1/L2)
- Dropout layers
- Cross-validation
- Data augmentation

Dependency on Large, High-Quality Datasets

Most powerful AI models (e.g., GPT, BERT, vision transformers) are data-hungry.

Quality and bias in training data directly affect model performance and fairness.
Issues include:

- Expensive and time-consuming data labeling
- Data privacy concerns
- Underrepresentation of minority groups

Integration of Domain Knowledge

Purely data-driven models can ignore well-established **domain-specific rules**. Research aims to blend:

- **Symbolic AI** (logic-based systems)
- **Neural networks** (learning from data)
- This **hybrid approach** can improve:
- Interpretability
- Data efficiency
- Trustworthiness of AI systems

Hybrid Models with Mathematical Interpretability

- These models aim to:
- Preserve the strengths of AI (e.g., pattern recognition, adaptability)
- Retain **analytical rigor** and **theoretical transparency** of traditional models
- Examples include:
- Physics-informed neural networks (PINNs)
- Neural ODEs (Ordinary Differential Equations)
- Probabilistic graphical models with neural components

Future Directions

Future work may focus on:

- Explainable AI to enhance trust and transparency in AI-driven models.
- Integration of symbolic reasoning with neural methods.
- Development of frameworks that combine mechanistic and data-driven approaches.

VI. CONCLUSION

AI is reshaping the landscape of mathematical modelling, providing tools to model complex systems more effectively. While challenges remain, the integration of AI into modelling frameworks holds great promise for advancing both theoretical understanding and practical applications.

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