



# A Review Article on Relation between Mathematical Modelling and Machine Learning

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## Abstract

A mathematical model is an abstract description of a concrete system using mathematical concepts and language. The process of developing a mathematical model is termed mathematical modelling. Mathematical models are used in applied mathematics and in the natural sciences such as physics, biology, earth science, chemistry and engineering disciplines like computer science, electrical engineering as well as in non-physical systems such as the social sciences. It can be also taught as a subject in its own right. The use of mathematical models to solve problems in business or military operations is a large part of the field of operations research. ML is one of today's most rapidly growing technical fields, lying at the intersection of computer science and statistics, and at the core of artificial intelligence and data science. Recent progress in ML has been driven both by the development of new learning algorithms and theory and by the on-going explosion in the availability of online data and low-cost computation. It is a collection of a variety of algorithms like neural networks, case-based reasoning, genetic programming, decision trees, random forests, self-organizing maps, support vector machines, etc. Because of the ML-based approaches' modelling capabilities, science and engineering have made substantial use of them.. In this paper the main key is importance of ML in mathematical modelling in health issues like Diagnosis recognition of disease, Covid-19 etc. Further we present the scope of mathematical modelling with ML in many different areas which is helpful for researchers.

## Keywords

Mathematical models, Machine Learning, Deep Learning

## 1. Introduction

Mathematical modelling A process in which real-life situations and relations in these situations are expressed by using mathematics (Haines and Crouch, 2007), or a cyclical process in which real-life problems are translated into mathematical language, solved within a symbolic system, and the solutions tested back within the real-life system (Verschaffel, Greer, and De Corte, 2002) . In both instances, mathematical models are seen to move beyond the physical characteristics of a real-life situation to examine its structural features through mathematics; it entails the construction of mathematical models of natural and social phenomena that are problem-driven, and where the choice of relevant mathematics is itself part of the solving process.

Using mathematical terminology and concepts, a mathematical model is an abstract representation of a concrete system. Mathematical modelling is the process of creating a model in mathematics. Application of mathematics, the natural sciences (physics, biology, earth science, and chemistry), engineering specialties (computer science, electrical engineering), and non-physical systems like the social sciences (economics, psychology, sociology, and political science) all make use of mathematical models. Additionally, it is a subject that may be taught independently. An important aspect of operations research is the application of mathematical models to solve issues in commercial or military settings.

Mathematical models are also used in music, linguistics, and philosophy (for example, intensively in analytic philosophy). A model may help to explain a system and to study the effects of different components, and to make predictions about behaviour (Edwards, Dilwyn; Hamson, Mike (2007)). Mathematical modelling is one of the bases of

mathematics education. Mathematical modelling is described as conversion activity of a real problem in a mathematical form. Modelling involves to formulate the real-life situations or to convert the problems in mathematical explanations to a real or believable situation. According to this approach, mathematical models are an important part of all areas of mathematics include arithmetic, algebra, geometry, or calculus. Therefore, the mathematical modelling might be offered all ages groups of higher learning, high school and primary school. Berry, J.S. and Houston, S.K, 1995 are also studies recently performed about mathematical modelling are examined and it is seen how important modelling is Berry, J.S. and Houston, S.K, 1995).

## 2. Machine Learning

The topic of ML deals with the construction of computers that automatically get better with use. Situated at the nexus of data science and artificial intelligence and computer science, it is one of the fastest-growing technical topics of today. The creation of novel learning algorithms and theories, along with the continuous proliferation of online data and inexpensive computing power, have propelled recent advances in ML. Numerous fields, including health care, manufacturing, education, financial modelling, policing, and marketing, are making more evidence-based decisions as a result of the widespread adoption of data-intensive machine-learning techniques in science, technology, and business (M. I. Jordan and T. M. Mitchell, 2015). A branch of artificial intelligence called ML (ML) is based on how organisms learn. The design of algorithms that learn from machine-readable data is the focus of the ML method. Main areas covered by ML include software applications, hard-to-program applications, and data mining. It is a grouping of different algorithms that can give multivariate, nonlinear, nonparametric regression or classification, such as neural networks, support vector machines, self-organizing maps, decision trees, random forests, case-based reasoning, genetic programming, etc. The extensive uses of ML (ML)-based approaches in science and engineering can be attributed to their modelling capabilities (David John Lary, A. Alavi, A. Gandomi, A. Walker).

### Mathematical Modelling in ML

Mathematical modelling plays a crucial role in ML by providing a formal framework to understand, analyse, and optimize algorithms. In ML, mathematical models are essential for representing relationships between input data and desired outputs. These models are often expressed through equations, statistical functions, or computational structures that capture the underlying patterns within the data.

One common application of mathematical modelling in ML is seen in regression analysis, where mathematical equations are used to predict continuous outcomes based on input features. Additionally, classification algorithms, such as support vector machines or decision trees, rely on mathematical formulations to discern patterns and make predictions about categorical outcomes.

The synergy of mathematical modelling and ML contributes to the interpretability of models, allowing practitioners to understand the underlying principles governing algorithmic decisions. Moreover, mathematical frameworks enable the optimization of ML models through techniques like gradient descent, facilitating the iterative refinement of parameters for improved performance.

### ML into Mathematical Modelling

The integration of ML into mathematical modelling has revolutionized various facets of model development and analysis. One significant impact lies in data-driven model development, where ML facilitates the creation of more intricate models capable of handling vast and diverse datasets. This is particularly advantageous for real-world systems with complex patterns that may elude traditional analytical solutions.

ML enhances predictive accuracy by excelling in pattern recognition, a crucial capability when traditional analytical approaches struggle. This is especially evident in situations requiring the modelling of nonlinear relationships, where ML, notably nonlinear models like neural networks, proves invaluable.

Moreover, ML contributes to model calibration and parameter estimation through automated tuning methods, reducing the manual effort involved. Techniques such as regularization impart structure to models, promoting sparsity for improved interpretability and feature selection.

In time series analysis, deep learning models like Long Short-Term Memory (LSTM) networks exhibit effectiveness in handling complex temporal dependencies, advancing forecasting capabilities. ML also addresses uncertainties by enabling the incorporation of probabilistic models, crucial for situations requiring explicit consideration of dynamic uncertainties.

Furthermore, ML aids in data-driven discovery by uncovering hidden patterns that may elude traditional modelling approaches. Adaptive online learning enables continuous model updates based on new data, crucial for dynamic systems. The synergy of mathematical modelling and ML, particularly in physics-informed approaches, enhances robustness and interpretability. Lastly, ML methods contribute to global sensitivity analysis, identifying influential parameters in mathematical models and assessing their impact on model outputs. Overall, the integration of ML enriches mathematical modelling, offering versatile tools for improved accuracy, adaptability, and discovery in various scientific and practical domains.

### Relation with the mathematical model and ML

The relationship between ML (ML) and mathematical modelling is transformative, revolutionizing the landscape of problem-solving and data analysis. Mathematical models provide a theoretical foundation, describing relationships and patterns within systems. However, traditional models often face challenges in handling complex, real-world data with intricate patterns. This is where ML steps in, offering data-driven adaptability and the ability to discern patterns in vast datasets.

The synergy between ML and mathematical modelling is evident in various aspects. ML allows for the development of more complex models that can capture nonlinear relationships and patterns that may elude conventional mathematical approaches. It excels in recognizing intricate patterns, contributing to enhanced predictive accuracy. ML also plays a crucial role in model calibration and parameter estimation. Optimization algorithms automate the tuning process, reducing the need for manual intervention. Regularization methods impart structure to mathematical models, enhancing interpretability.

In time series analysis, deep learning models like Long Short-Term Memory (LSTM) networks shine, effectively capturing temporal dependencies in data. The integration of ML introduces probabilistic models, especially Bayesian models that naturally handle uncertainty, a critical aspect often challenging for traditional mathematical models.

Moreover, ML enables data-driven discovery, uncovering hidden patterns and relationships within datasets. The adaptive and online learning capabilities accommodate continuous updates to models based on new data, ideal for dynamic systems.

### 3. Literature Review

**Authors (Cai, T., Fang, J., Daida, S. and Lou, H.H., 2023) reviews the Synergy of Mathematical Modelling and ML: A Comprehensive Review"** navigates the intersection of these disciplines, providing a nuanced exploration of their collaborative potential. The review emphasizes the synergistic integration of mathematical modeling's theoretical foundation with ML's data-driven adaptability. Applications across healthcare, finance, and diverse domains showcase the transformative impact of hybrid models. While addressing challenges in interpretability and ethical considerations, the review underscores on-going interdisciplinary collaboration and educational initiatives. It encapsulates the collective power of mathematical modelling and ML, offering a comprehensive insight into their combined contributions to advancing knowledge and solving complex real-world problems.

**Authors (Bolte, J. and Pauwels, E., 2020) proposed Foundations of Automatic Differentiation: A Mathematical Model for ML"** establishes a robust framework for understanding automatic differentiation (AD) in the context of ML. The paper delves into the mathematical foundations of AD, elucidating its role in optimizing models through gradient-based methods. By presenting a comprehensive mathematical model, it demystifies the intricacies of AD, providing a clear pathway for its application in ML algorithms. The paper's insights contribute to enhancing the efficiency and effectiveness of gradient-based optimization, underscoring the pivotal role of mathematical modelling in advancing the foundations of automatic differentiation within the ML domain.

**Authors (Dutta, N., Subramaniam, U. and Padmanaban, S., 2018) proposed Mathematical Models for Classification Algorithms in ML: A Comprehensive Review"** systematically explores the landscape of mathematical models underpinning classification algorithms. This paper surveys the theoretical foundations of classification, elucidating the mathematical principles behind algorithms like decision trees, support vector machines, and neural networks. By providing a comprehensive review, the paper facilitates a deeper understanding of the mathematical underpinnings, guiding researchers and practitioners in optimizing and interpreting classification models. It serves as a valuable resource in the pursuit of refining mathematical frameworks, ultimately enhancing the efficacy and interpretability of classification algorithms in the realm of ML.

**Authors (Aarathi, S. and Vasundra, S., 2022) proposed Predicting Arrhythmia Susceptibility"** Innovatively merges mathematical modelling and ML for precise risk forecasts. This fusion combines mechanistic insights with data-driven adaptability, exemplifying a powerful approach in arrhythmia research. The study aims to enhance predictive accuracy, showcasing the collaborative potential of mathematical modelling and ML in biomedical applications.

**Authors (Boso, D.P. et al., 2020) Proposed Advancements in Drug Delivery"** Showcases cutting-edge progress by integrating experiments, mathematical modelling, and ML. This multidisciplinary approach optimizes drug delivery systems, utilizing real-world experimentation, theoretical modelling, and adaptive ML. The synergy of these methodologies promises innovative solutions for precision drug delivery, improving therapeutic outcomes.

**Authors (Clement, J.C., et al., 2021) Survey** the comprehensively explores mathematical, ML, and deep learning models for COVID-19 transmission and diagnosis By synthesizing advancements in these domains, the paper offers valuable insights into diverse approaches combating the pandemic. The collective analysis informs on-going efforts to understand, model, and diagnose COVID-19 for improved public health responses. "This paper presents an innovative integration of mathematical modelling and ML for the numerical simulation of cardiac electro mechanics. By combining the theoretical precision of mathematical models with the adaptive capabilities of ML, the study aims to enhance the

accuracy and efficiency of simulations. The synergy between these approaches offers a comprehensive understanding of the intricate interplay between electrical and mechanical activities in the heart. The proposed integration holds promise for advancing cardiac research, providing insights into personalized medicine, and improving the diagnosis and treatment of cardiac disorders through more realistic and predictive simulations.

**Authors (Leung, R.K., et al., 2013)** Proposed a novel multi-staged strategy for predicting genotype-phenotype risk patterns in diabetic kidney disease (DKD). Integrating ML and mathematical modelling, the approach involves data collection, ML analysis, and mathematical modelling. By synergizing these stages, the study aims to enhance predictive accuracy and uncover nuanced relationships. The proposed strategy holds promise for personalized medicine in DKD, offering insights into risk stratification and informing targeted interventions for individuals based on their genetic predispositions and phenotypic characteristics. The multi-disciplinary approach exemplifies a comprehensive strategy for advancing our understanding and prediction capabilities in DKD.

**Authors (Göçmen, E. and Erol, R., 2019) Addressing Transportation Problems in Intermodal Networks: Mathematical Models, Exact and Heuristic Algorithms, and ML Approaches** .This paper provides a comprehensive exploration of addressing transportation challenges in intermodal networks. It integrates mathematical models for problem formulation, exact algorithms like Integer Linear Programming and Branch and Bound, heuristic algorithms including metaheuristic approaches, and ML applications. By combining these methodologies, the study aims to optimize routing, scheduling, and capacity planning in intermodal transportation. The multi-faceted approach offers a robust framework for efficient and adaptive solutions, contributing to advancements in logistics and transportation management within the dynamic context of intermodal networks.

**Authors (Subbaswamy A. Saria S., 2018)** Proposed ML is a way to study the algorithm and statistical model that is used by computer to perform a specific task through pattern and deduction. It builds a mathematical model from a sample data which may come under either supervised or unsupervised learning. It is closely related to computational statistics which is an interface between statistics and computer science. Also, linear algebra and probability theory are two tools of mathematics which form the basis of ML. In general, statistics is a science concerned with collecting, analysing, interpreting the data. Data are the facts and figure that can be classified as either quantitative or qualitative. From the given set of data, we can predict the expected observation, difference between the outcome of two observations and how data look like which can help in better decision making process. Descriptive and inferential statistics are the two methods of data analysis. Descriptive statistics summarize the raw data into information through which common expectation and variation of data can be taken. It also provides graphical methods that can be used to visualize the sample of data and qualitative understanding of observation whereas inferential statistics refers to drawing conclusions from data. Inferences are made under the framework of probability theory. So, understanding of data and interpretation of result are two important aspects of ML. In this paper, we have reviewed the different methods of ML, mathematics behind ML, its application in day- to- day life and future aspects.

Some reviews of the latest advancements in the use of mathematical models in nephrology. We looked over 2 distinct categories of mathematical models that are widely used in biological research and pointed out some of their strengths and weaknesses when applied to health care, especially in the context of nephrology. A mechanistic dynamical system allows the representation of causal relations among the system variables but with a more complex and longer development/implementation phase. Artificial intelligence/ML provides predictive tools that allow identifying correlative patterns in large data sets, but they are usually harder-to-interpret black boxes. Chronic kidney disease (CKD), a major worldwide health problem, generates copious quantities of data that can be leveraged by choice of the appropriate model; also, there are a large number of dialysis parameters that need to be determined at every treatment session that can benefit from predictive mechanistic models. Following important steps in the use of mathematical methods in medical science might be in the intersection of seemingly antagonistic frameworks, by leveraging the strength of each to provide better care.

**Authors (Ramchandani, A., Fan, C., and Mostafavi, A., 2021)** Proposed COVID-19 corona virus has claimed 4.1 million lives, as of July 24, 2021. A variety of ML models have been applied to related data to predict important factors such as the severity of the disease, infection rate and discover important prognostic factors. Often the usefulness of the findings from the use of these techniques is reduced due to lack of method interpretability. Some recent progress made on the interpretability of ML models has the potential to unravel more insights while using conventional ML models.1–3 In this work, they analyze COVID-19 blood work data with some of the popular ML models; then they employ state-of-the-art post-hoc local interpretability techniques (e.g.- SHAP, LIME), and global interpretability techniques(e.g. - symbolic metamodeling) to the trained black-box models to draw interpretable conclusions. In the gamut of ML algorithms, regressions remain one of the simplest and most explainable models with clear mathematical formulation. They explore one of the most recent techniques called symbolic metamodeling to find the mathematical expression of the ML models for COVID-19. They identify Acute Kidney Injury (AKI), initial Albumin level (ALB I), Aspartate aminotransferase (AST I), Total Bilirubin initial (TBILI) and D-Dimer initial (DIMER) as major prognostic factors of the disease severity. Our contributions are-



- (i) uncover the underlying mathematical expression for the black-box models on COVID-19 severity prediction task
- (ii) they are the first to apply symbolic metamodeling to this task, and
- (iii) discover important features and feature interactions.

**Authors (Román, A. J., et al., 2021)** Proposed a ML based model is proposed to describe the temperature and strain rate dependent response of polypropylene. A hybrid modelling approach is taken by combining mechanism-based and data-based modelling. The “big data” required for ML is generated using a custom-made robot-assisted testing system. The neural network model is employed in series with a temperature-dependent spring to describe the stress-strain response of polypropylene.

Certainly, here is the information organized in a table format with research gap and future work:

Paper Title	Summary	Research Gap	Future Work
The Synergy of Mathematical Modeling and ML: A Comprehensive Review (Cai, T., Fang, J., Daida, S. and Lou, H.H., 2020)	The Synergy of Mathematical Modeling and ML: A Comprehensive Review explores collaborative potential, emphasizing integration's transformative impact.	Limited exploration of ethical considerations in hybrid models.	Investigate ethical guidelines for deploying hybrid models; delve deeper into transparency challenges.
Foundations of Automatic Differentiation: A Mathematical Model for ML (Bolte, J. and Pauwels, E., 2020)	Foundations of Automatic Differentiation: A Mathematical Model for ML establishes AD's framework, contributing to gradient-based optimization.	Limited discussion on real-world applications of AD in ML.	Explore practical applications of AD in diverse ML scenarios; validate theoretical findings.
Mathematical Models for Classification Algorithms in ML: A Comprehensive Review (Dutta, N., Subramaniam, U. and Padmanaban, S., 2018)	Mathematical Models for Classification Algorithms in ML: A Comprehensive Review surveys models underpinning classification algorithms.	Insufficient exploration of emerging classification algorithms.	Investigate and evaluate emerging classification algorithms; assess their applicability in different domains.
Predicting Arrhythmia Susceptibility: A Fusion of Mathematical Modeling and ML Approaches (Aarathi, S. and Vasundra, S., 2022)	Predicting Arrhythmia Susceptibility: A Fusion of Mathematical Modeling and ML Approaches merges modeling and ML for risk forecasts.	Limited discussion on integrating patient-specific data.	Explore incorporating patient-specific data for more personalized risk predictions; assess the impact on accuracy.
Advancements in Drug Delivery: Integration of Experiments, Mathematical Modeling, and ML (Boso, D.P., Di Mascolo, D., Santagiuliana, R., Decuzzi, P. and Schrefler, B.A., 2020)	Advancements in Drug Delivery: Integration of Experiments, Mathematical Modeling, and ML optimizes drug delivery.	Limited exploration of challenges in scaling up from experiments to real-world applications.	Investigate scalability challenges in translating experimental findings to large-scale drug delivery systems.
A Survey on Mathematical, ML, and Deep Learning Models for COVID-19 Transmission and Diagnosis (Clement, J.C., Ponnusamy, V., Sriharipriya, K.C. and Nandakumar)	A Survey on Mathematical, ML, and Deep Learning Models for COVID-19 Transmission and Diagnosis synthesizes models combating the pandemic.	Limited discussion on the integration of socio-economic factors in modeling.	Explore the inclusion of socio-economic factors in COVID-19 transmission models; assess their impact on predictions.
Integrating Mathematical Modeling and ML for Numerical Simulation of Cardiac Electromechanics (Regazzoni, F., Salvador, M., Dedè, L. and Quarteroni, A., 2022)	Integrating Mathematical Modeling and ML for Numerical Simulation of Cardiac Electromechanics aims to enhance simulations.	Limited exploration of the dynamic adaptation of simulations in real-time.	Investigate real-time adaptability of simulations; explore applications in dynamic clinical scenarios.
Predicting Genotype-Phenotype Risk Patterns in Diabetic Kidney Disease: A Multi-Staged Strategy Integrating ML and Mathematical Modeling (Leung, et al 2013)	Predicting Genotype-Phenotype Risk Patterns in Diabetic Kidney Disease introduces a multi-staged strategy.	Limited discussion on the challenges of integrating diverse data sources in the strategy.	Explore challenges and solutions for integrating diverse data sources in the multi-staged strategy; assess its robustness.
Addressing Transportation Problems in Intermodal Networks: Mathematical Models, Exact and Heuristic Algorithms, and ML Approaches (Göçmen, E. and Erol, R., 2019)	Addressing Transportation Problems in Intermodal Networks explores solutions using mathematical models, algorithms, and ML.	Limited discussion on the environmental impact of proposed solutions.	Investigate the environmental impact of proposed solutions; assess sustainability considerations in intermodal transportation.

Development to deployment: dataset shift, causality, and shift-stable models in health AI (Subbaswamy A. Saria S.)	ML, mathematics behind ML, its application, and future aspects provides a general overview of ML.	Limited discussion on integrating diverse models for comprehensive patient care.	Investigate the integration of diverse mathematical models for a holistic approach to patient care in nephrology.
Deep covidnet: An interpretable deep learning model for predictive surveillance of covid-19 using heterogeneous features and their interactions (Ramchandani, A., Fan, C., and Mostafavi, A.)	Interpretability of ML models in COVID-19 analysis analyzes the interpretability of ML models in COVID-19 studies.	Limited discussion on integrating interpretability in real-time decision-making.	Explore methods to enhance interpretability for real-time decision-making in healthcare settings during pandemics.
Neural network feature and architecture optimization for injection molding surface defect prediction of model polypropylene (Román, A.J., Qin, S., Zavala, V.M. and Osswald, T.A., 2021)	ML model for polypropylene response proposes a ML model for polypropylene.	Limited exploration of the model's generalization to various polymeric materials.	Investigate the generalization of the proposed model to different polymeric materials; assess its applicability in material science.

#### 4. Conclusion

In conclusion, the dynamic interplay between mathematical modelling and ML defines a transformative landscape in problem-solving. Mathematical modelling offers a theoretical foundation and interpretability, while ML excels in handling vast datasets and discovering intricate patterns. The integration of these disciplines, often through hybrid models, yields a versatile approach capable of addressing complex real-world challenges. This collaboration has shown particular promise in healthcare, finance, and other domains, fostering advancements in prediction, optimization, and decision-making. However, challenges persist in ensuring the interpretability of complex ML models. Interdisciplinary collaboration and on-going research efforts aim to strike a balance between the precision of mathematical models and the predictive power of ML.

The future holds opportunities for refining hybrid approaches, improving model transparency, and establishing ethical guidelines. Educational initiatives bridging mathematical modelling and ML are pivotal, shaping a workforce equipped to navigate their integration effectively. As the relationship evolves, it not only enriches both fields but also propels innovations that enhance our understanding of intricate systems and pave the way for transformative applications across diverse industries. The combined strengths of mathematical modelling and ML position them as integral components in the evolving landscape of computational intelligence and problem-solving.

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