

Machine Learning in Nonlinear Material Physics

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DOI: <https://doi.org/10.30880/jscdm.2024.05.01.010>

Article Info

Received: 1 December 2023
Accepted: 25 April 2024
Available online: 21 June 2024

Keywords

Machine learning, data mining, continuum materials mechanics, materials science, predictive modeling, prescriptive modeling, neural networks, microstructure, mechanical properties, performance evaluation

Abstract

Researchers and investors can accelerate the development of innovative materials, methods, and procedures by using machine learning technologies. In materials science, one key objective of employing such methods is to make it easier to identify and quantify high features throughout the chain of manipulation, organization, possessions, and efficiency. An overview of effective uses of automated learning and statistics is given in this piece, which addresses specific challenges in continuous materials mechanics. The classification of these applications is based on their nature, categorized as descriptive, predictive, or prescriptive, all aiming to identify, anticipate, or optimize crucial attributes. The selection of the most suitable machine learning technique is influenced by factors such as the unique use case, content type, data characteristics, geographical and temporal scales, formats, targeted knowledge gain, and affordable computing expenses. Various examples are explored, including using various artificially generated share network architectures on an as-needed basis in conjunction with additional data-driven approaches such as basic constituent assessment, decisions shrubs, models, woods, trees, supported matrix, and Gaussian learners.

1. Introduction

The application of machine learning techniques in continuous materials mechanics is driven by the potential to expedite and streamline the discovery and development of new materials for future applications [1]. The significant challenge lies in manipulating material qualities to achieve a desirable blend of features and performance attributes. The primary goals in developing materials for specific applications involve detecting linked physical events across various spatiotemporal scales, addressing statistical errors, and regulating the parameter space within materials structures [2]. It is crucial to consider the statistical variation of the current process to connect the impacts of process settings to microstructural traits, material qualities, and performance characteristics across different scales. Additionally, data mining assists scientists in exploring and comprehending intricate nonlinear interactions at a fundamental level [3-6].

Data mining and machine learning techniques are frequently employed as stepping stones in addressing complex issues until the nature of the connection of interest can be encapsulated by more general physical models replacing the learned algorithms. There is exceptional potential to objectively calibrate unexpected model forms

and parameters in physics-based models through machine learning techniques grounded in rigorous statistical methods [7]. Methodologically, the fields of machine learning and data mining, components of the data science toolkit, are closely connected to applied statistics, and their distinctions are intertwined [8]. The cross-industry standard outlines step in data mining, including issue comprehension, data understanding, data preparation, modeling, data evaluation using machine learning, and implementing trained algorithms. Data mining and machine learning methods involve training, testing, and verifying implemented algorithms, along with proper pre-processing of relevant data [9, 10]. Consequently, the prescriptive goal of optimization is often achieved through post-learning activities like feature optimization and decision-making [11].

The literature offers various database methodologies to address challenges within continuous materials mechanics (Figure 1). Our approach encompasses issues throughout the process-structure-property-performance chain, considering diverse data dimensions across geographical and temporal scales. To systematically study data mining and machine learning methods, we've categorized them into four primary areas based on application fields: performance, microstructure, mechanical characteristics, and process parameters. Within each area, topics are further classified into three categories—descriptive, predictive, and prescriptive—depending on the type of machine learning and data mining activity and the goal pursued.

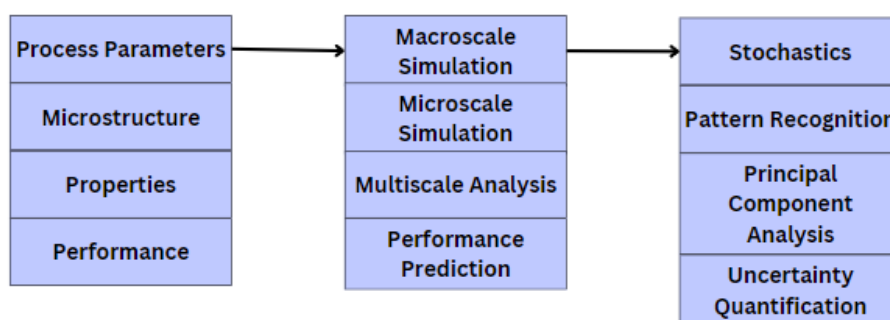


Fig. 1 Classification of the system

This difference was first put out by Delen and Ram [12], mainly for use in business intelligence. Researchers investigated and divided data mining tasks between basic and authoritarian groups. On the other hand, to address practical enhancements in chemical biomechanics and process-structure-property-performance links, we provide a proactive machines intelligence task section. Thus, our adopted hierarchy offers a comprehensive framework for examining various methodologies in this review.

This analysis includes an initial compilation of descriptions of key machine learning techniques, which can be used independently or in combinations across diverse research. As Witten et al. emphasize, it's important to note that no single machine-learning approach is universally suitable for all data mining tasks [13-15]. The notion of the ubiquitous learner, according to their experience, remains a utopian fiction.

The field of machine learning is currently in its nascent stages, undergoing constant evolution. Despite many techniques and algorithms for years, recent developments have brought forth new approaches, shaping machine learning into a fresh and continually developing discipline [16, 17]. Precisely defining what machine learning entails remains challenging due to its dynamic nature. Data-driven methodologies are permeating various fields, including materials science, where specific problems and diverse data profiles have catalyzed the creation of novel variations and customized machine learning techniques. It is crucial not to underestimate the significance of "mainstay methods" in machine learning, particularly neural networks (ANNs) comprised of computers [18-20]. These networks, theoretically universal and flexible enough to approximate any function within data, maintain their importance despite evolving methodological landscapes (figure 2). While continuous changes are expected in the coming years, the approaches outlined in this chapter do not provide an exhaustive list of machine learning techniques practical for materials mechanics. Data science approaches are concurrently complementing and integrating with traditional materials science research procedures [21-23].

In this specific application, ANNs emerge as the most frequently encountered type of machine learning. Originating from the basic 1958 predecessor formulation known as the perceptron, ANNs have gained increasing popularity as the limitations that once impeded their use—specifically, increasing processing power and data availability have been overcome. Initially designed as a simple one-layer ANN, the perceptron functioned as a linear predictor [24-27].

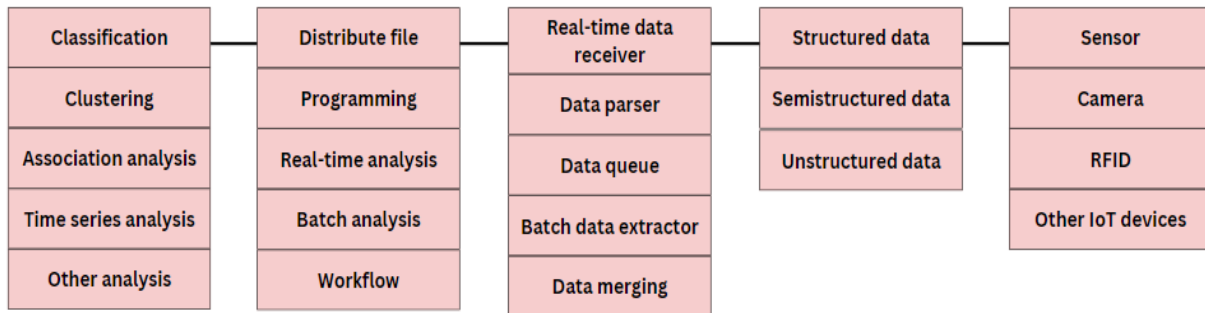


Fig. 2 Architecture of the system

ANNs offer specialized memory neurons/units that effectively address the vanishing gradient problem, a common issue leading to sub-optimal local minima, especially with increasing neural layers. Long Short-Term Memory (LSTM) networks, derived from ANNs, have gained popularity alongside deep learning architectures to overcome local entrapments in deep learning [28, 29]. In essence, LSTMs allow for greater information storage by "saving" relevant data points over time, preventing them from being drowned out and dispersing their error corrective signal across longer periods [30].

Randomized neural networks, providing individual neurons with random excitatory or inhibitory spikes, and radial basis ANN, essentially shallow Feedforward Neural Networks (FFNNs) using radial basis functions for individual neuron specialization, are essential to discuss [31].

2. Proposed Methodology

Machine learning is still in its infancy and constantly evolving in scientific research [32]. Although various methods and algorithms have existed for some time, recent advances have enhanced machine learning, making it a dynamic field that is constantly activating and changing. Because machine learning is constantly growing, it is difficult to pinpoint a specific definition of machine learning. Data-driven approaches have been integrated into a variety of fields, including materials science, leading to creative modifications and specialized machine learning techniques suited to specific problems and different data profiles

3. Algorithm

It is crucial not to underestimate the significance of foundational machine learning methods, exemplified by ANNs composed of interconnected computers [33]. These ANNs, theoretically versatile enough to approximate any function inherent in data, should not have their importance diminished by methodological domain-specificity [34]. Although we anticipate continuous changes in the coming years, the approaches outlined in this discourse cannot be considered an exhaustive list of machine learning techniques practical for materials mechanics (Figure 3). This is because data science approaches are designed to complement and integrate with traditional materials science research procedures.

- Step 1: Identify key areas within continuum materials mechanics where machine learning and data mining techniques are applied.
- Step 2: Collect relevant literature and research papers on the use of machine learning and data mining in continuum materials mechanics.
- Step 3: Review common datasets used in continuum materials mechanics research, including material properties, experimental data, and simulation results.
- Step 4: Analyze different machine learning and data mining algorithms employed for tasks such as material property prediction, microstructure characterization, and material behavior modeling.
- Step 5: Evaluate the strengths and limitations of machine learning and data mining approaches compared to traditional continuum mechanics methods.
- Step 6: Investigate challenges such as data scarcity, model interpretability, and computational efficiency when applying machine learning in continuum materials mechanics.
- Step 7: Explore hybrid approaches combining physics-based models with machine learning techniques to enhance predictive accuracy and physical interpretability.
- Step 8: Assess the impact of machine learning and data mining on advancing understanding and prediction capabilities in continuum materials mechanics.
- Step 9: Identify emerging trends and future research directions for integrating machine learning and data mining in continuum materials mechanics.

Step 10: Synthesize findings from the review to provide insights for researchers and practitioners aiming to leverage machine learning and data mining in continuum materials mechanics applications.

ANNs, particularly the well-known perceptron from 1958, have become the most prevalent form of machine learning in specific applications. Originally conceived as a simple one-layer ANN, the perceptron functioned as a linear predictor [235, 36]. Modern FFNNs are essentially multilayer perceptron's with connected vertices, allowing a "feedforward" signal to pass through the network in one direction.

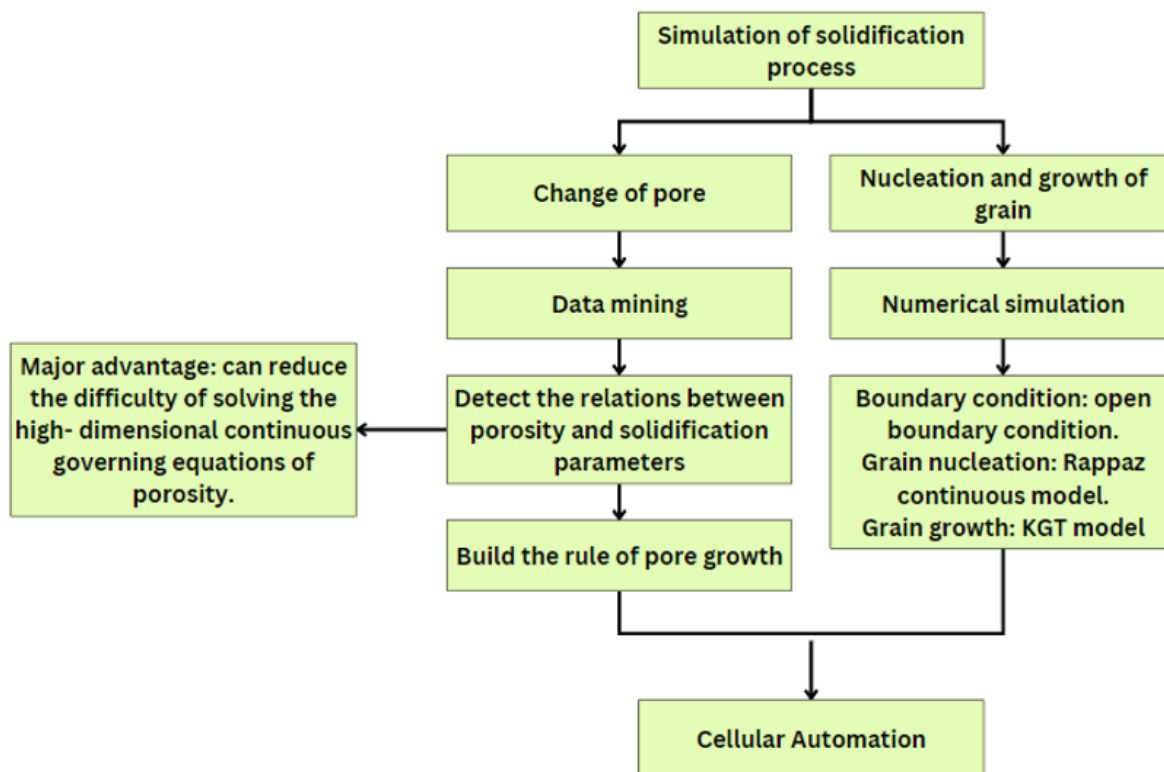


Fig. 3 Workflow methodology of the system

As the signal passes through the layers, it gradually changes from input to output. These networks typically use backpropagation gradient descent error reduction approaches that address issues such as local minima, activation function selection, overfitting, optimal number of layers and neurons, and network interpretability [37]. The difficulties associated with further study of ANNs must be recognized and overcome. These difficulties include overfitting, avoiding local minima, choosing appropriate activation functions, determining the optimal number of layers and neurons for each layer, and making the network understandable to people. They are not limited to these. These methods need to be continually improved to get the most out of machine learning in materials science and other scientific fields. Specialized memory neurons or units have emerged in the field of ANN as a potential solution to the vanishing gradient problem. Suboptimal local minima often result from this problem, especially as the number of neural layers' increases.

These techniques enable directed loops within the ANN topology, fostering communication that oscillates and overlaps with the processing of subsequent samples, facilitating data transfer across sequence stages in a purposeful manner [38]. While each technique discussed is primarily used individually in the context of materials science, it is anticipated that future developments will witness increased utilization of these techniques in tandem. They may be integrated into sequential serial learning pipelines, combining methods like clustering for feature selection with convolutional neural networks (CNNs) for subsequent feature learning, or incorporated into ensemble techniques where each approach contributes to a collective prediction [39, 40].

4. Microstructure

Extensive research has been conducted on microstructural quantification, categorization, evolution, and reconstruction, leading to a wealth of published findings [41]. Bridging length scales around the microstructure can be achieved through various methods, such as top-down approaches like localization or bottom-up methods like homogenization [42]. Additionally, this endeavor employs prescriptive, predictive, and descriptive methods, as shown in Figure 4. Descriptive identification of links between process parameters, generated microstructures,

resulting mechanical properties, and related fatigue events and failure mechanisms enables the prediction and prescriptive tailoring of microstructural features for optimization.

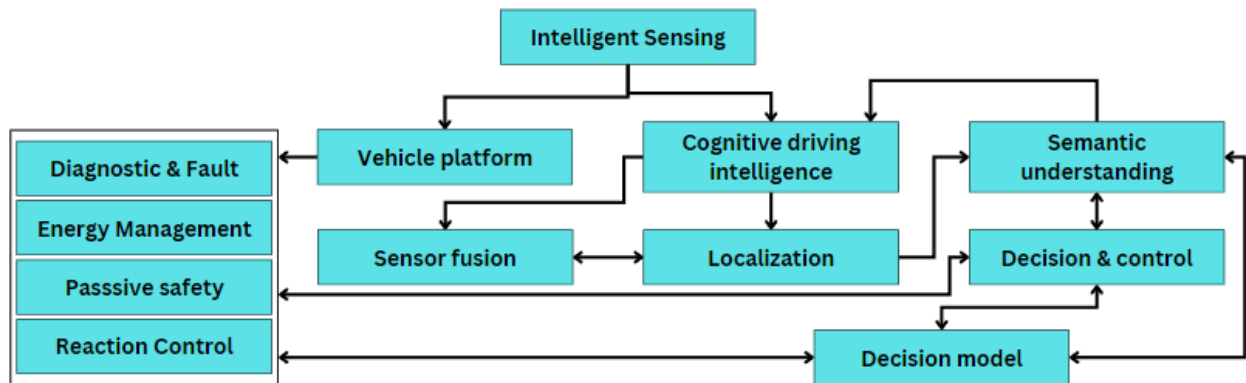


Fig. 4 Implementation of the system

A newly created nanoscale producer created a large collection of porous objects with various characteristics. Research findings measured the real porous wall shape using high-quality X-ray ultrasonography. We calculated and contrasted Bayesian formulations for both modeled and real cell structures using Principal Component Analysis (PCA) of two-point spatial connections, providing an objective measure of the variation between distinct datasets. This led to the quantification of porous membrane architectures and the acquisition of low-dimensional representations through PCA on these two-point statistics [43]. Key characteristics, such as the stretching factor, stretching direction, porosity, and pore size, were identified as the foundation of the low-dimensional space. Linkages between a broad range of microstructure properties and their impact on the low-dimensional space facilitated accurate estimations of the actual membrane characteristics using the basis matrix and the main component value [44].

The primary objective was to expand the application of the statistical continuum theory-based prior linking approach to accommodate greater elastic contrasts in composition, overcoming previous applicability constraints. Constructing a predictive model involves two main components: regression and feature extraction, both crucial in establishing correlations. To evaluate the data-driven predicting model's effectiveness for localization, three test scenarios were explored.

5. Mechanical Properties

The accurate anticipation and control of mechanical material qualities are imperative as they are closely intertwined with and significantly influenced by process variables and the resulting microstructures. Constitutive equations have traditionally been employed to elucidate mechanical behavior in simulations [45]. Prior to the recent surge in machine learning's popularity within the scientific community, various strategies, including ANN, were proposed to replace foundational equations with data-based techniques. Notable instances include approximating yield strength with consideration for specific technical obstacles in estimating the shear of elastic expansion and compression toughness of concrete elements and developing a super alloy using metal. Prescriptive instruction duties like enhancement, prediction tasks like grouping, and explanatory tasks like identifying patterns are often implemented in order to satisfy fundamental property needs for specific uses.

6. Performance Results

The performance of materials, particularly regarding fatigue and failure, becomes increasingly critical when subjected to stress over time. Specific material behaviors, such as fracture initiation, development, and formation under static and cyclic loads, dictate the material's behavior, leading to fatigue. Utilizing machine learning techniques to identify connections to fracture initiation, crack growth, and fatigue life performance is essential in selecting and developing optimal features throughout the process-structure-property-performance chain, as shown in Table 1.

Table 1 System features and their description, benefits and challenges

Feature	Description	Benefits	Challenges
Data sources:	Experimental data (e.g., stress-strain curves, microscopy images), simulation data (e.g., finite element models). And potentially property databases.	Rich information capturing material behavior across different scales and conditions.	Data quality and availability limitations, potential inconsistencies between sources, privacy concerns for proprietary data
Machine learning techniques:	Supervised learning (e.g., regression, classification) for predicting material properties, microstructure analysis, and failure prediction. Unsupervised learning (e.g., clustering dimensionality reduction) is used to identify material phases, hidden patterns, and anomalies.	Improved accuracy and efficiency compared to traditional methods, ability to learn complex relationships from large datasets	Model interpretability and explainability. Potential bias in algorithms and data, challenges in handling noisy and incomplete data
Data mining techniques:	Feature engineering dimensionality reduction and outlier detection to prepare data for machine learning and identify relevant information	Improved model performance by extracting meaningful features and reducing data complexity.	It requires domain knowledge and expertise for effective feature selection and potential loss of information in dimensionality reduction.
Multiscale modeling:	Combines data from different scales (microstructure, macroscale) through multiscale modeling frameworks to predict material behavior at various levels.	Enables a more accurate and complete understanding of material behavior across different length scales.	The complexity of multiscale models, challenges in data integration and computational cost
Material design and optimization:	Uses machine learning to design novel materials with desired properties, optimize manufacturing processes, and predict performance under specific conditions.	Accelerates material development and discovery and optimizes material performance for specific applications.	Ethical considerations regarding potential biases in design algorithms, ensuring transparency and fairness in material development.

Corrosion, another intricate process, is strongly influenced by the environment, mechanical stresses, and the composition and microstructure of the alloy [46]. Metallic biomaterials derived from magnesium alloys may biodegrade, necessitating careful planning of the deterioration rate of implants like screws and plates. This ensures that the implant supports the load until the bone sufficiently heals to bear mechanical loads. The challenge lies in the multitude of factors combined with the extended duration of a corrosion test [47]. A crucial discovery was that the quantity of CO₂ and the concentration of NaCl were the two primary variables governing the corrosion rate. While the former was widely known, our research highlighted the significance of the latter. This observation is especially crucial since the CO₂ content varies significantly between in vitro and in vivo tests. The trained ANN enables a quantitative estimation of the corrosion rate under given conditions, aiding in planning additional trials in specific regions of interest [48-49].

7. Discussion

In the realms of health monitoring and lifespan prediction for engineering structures, data has historically played a pivotal role. Recent advancements in Bayesian methods and artificial intelligence, particularly artificial neural networks, have inspired numerous articles presenting innovative data-driven methodologies for lifespan prediction [50-52].

Simulating the incubation life of the cracking process, particularly in a specific microstructure exposed to high fatigue stresses, revealed a proportional link between the diameter of included voids and anticipated fatigue performance, while the breadth of voids exhibited an inverse correlation to fatigue life.

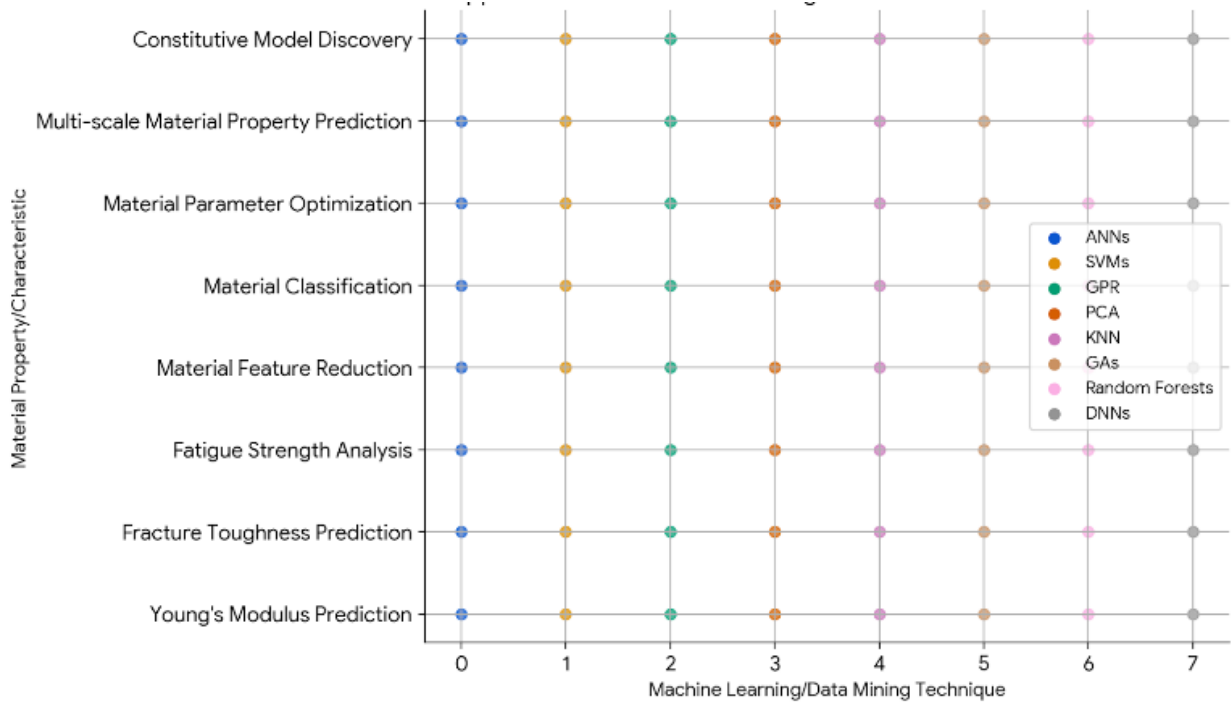


Fig. 5 Application of ML in continuum materials mechanics for the system

A deep neural network, specifically a graph segmentation network, was employed to identify fracture features within the material. Subsequently, a recurrent neural network modeled the evolution of these features. Training the system using a collection of time series graphs from 145 simulations allowed the concurrent prediction of the evolution of various material characteristics based on their initial conditions. Despite a 2% error in average fracture size prediction, a 13% error in damage size distribution, and an absolute error of 15% in the anticipated time to failure compared to equivalent simulation findings, the network demonstrated its capability. The network was further trained using previously generated inaccurate predictions to enhance accuracy, enabling it to learn from its errors and progressively minimize prediction errors.

8. Conclusion

In continuum solids mechanics, a diverse range of machine learning techniques has proven effective, independently or in various combinations. These techniques serve prescriptive, predictive, or descriptive purposes within the procedure, structure, attribute, and outcome chain. Accelerating item evaluation and synthesis is made possible using these approaches, commonly in a scale-bridging fashion. Integrating data science tools into established processes, such as combining classic constitutive model-based simulation tools with data-driven process learning and statistical techniques for data-driven simulations, is a promising approach. The synergy between data-based and physics-based modeling can yield hybrid analytics and simulations that are both reliable and efficient. Reinforcement learning, an intriguing technique, is promising for continuous materials mechanics. Particularly beneficial when decisions are integral to materials-related scenarios, reinforcement learning is a viable strategy in materials mechanics.

Acknowledgement

This project was supported by Nawroz University.

Conflict of Interest

Authors declare that there is no conflict of interests regarding the publication of the paper.

Author Contribution

All authors have contributed significantly to the research and writing of this paper, each bringing their unique expertise and insights to ensure the quality and comprehensiveness of the final manuscript.

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