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# Machine learning-based constitutive modelling for material non-linearity: A review

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**ABSTRACT**

Machine learning (ML) models are widely used across numerous scientific and engineering disciplines due to their exceptional performance, flexibility, prediction quality, and ability to handle highly complex problems if appropriate data are available. One example of such areas which has attracted a lot of attentions in the last couple of years is the integration of data-driven approaches in material modeling. There has been several successful researches in implementing ML-based constitutive models instead of classical phenomenological models for various materials, particularly those with non-linear mechanical behaviors. This review paper aims to systematically investigate the literature on ML-based constitutive models for materials and classify these models based on their suitability for material non-linearity including Non-linear elasticity (hyperelasticity), plasticity, visco-elasticity, and visco-plasticity. Furthermore, we also reviewed and compared the ML-based approaches that have been applied for architectured materials as these groups of materials are designed to represent specific material behaviors that might not exist in classical and conventional material categories. The other goal of this review paper is to provide initial steps in understanding of various ML-based approaches for material modeling, including artificial neural networks (ANN), Gaussian processes, random forests (RF), generated adversarial networks (GANs), support vector machines (SVM), different regression models and physics-informed neural networks (PINN). This paper also outlines different data collection methods, types of data, data processing approaches, the theoretical background of the ML models, advantage and limitations of various models, and potential future research directions. This comprehensive review will provide researchers with the knowledge necessary to develop high-fidelity, robust, adaptable, flexible, and accurate data-driven constitutive models for advanced materials.

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Data-driven material models; machine learning; material non-linearity; architectured materials; metamaterials

## Nomenclature

## Greek symbols

| | |
|---|---|
| ML | Machine Learning |
| ANN | Artificial Neural Networks |
| RF | Random Forests |
| GAN | Generated Adversarial Networks |
| SVM | Support Vector Machines |
| PINN | Physics-Informed Neural Networks |
| AI | Artificial Intelligence |
| MD | Molecular Dynamics |
| FEM | Finite Element Method |
| TBNN | Tensor Basis Neural Network |
| SPD-NN | Symmetric Positive Definite Neural Network |
| FFNN | Feed Forward Neural Network |
| ECNN | Equilibrium basis Convolution Neural Network |
| DMN | Deep Material Network |
| CANN | Constitutive Artificial Neural Network |
| DEM | Deep Energy Method |
| MSE | Mean Square Error |
| RMSE | Root Mean Square Error |
| LSTM | Long-Short Term Memory |
| GA | Genetic Algorithm |
| RSM | Response Surface Method |
| EPR | Evolutionary Polynomial Regression |
| NNO | Neural Network Optimization |
| IPA | Interior-Point Algorithm |
| RVM | Relevance Vector Machine |
| GPR | Gaussian Process Regression |
| KNN | K-Nearest Neighbor |

## 1. Introduction

Machine learning models, as a subset of Artificial Intelligence (AI), are speedily infiltrating numerous scientific and technological fields. This is due to the outstanding performance of data analytics and computing models beyond human capacity. Researchers in several disciplines of science use a variety of methods to address the challenges posed by growing data volumes. Therefore, ML is gaining prominence in

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various fields of engineering, including but not limited to: biomedical engineering [1] advanced digital manufacturing [2], autonomous driving vehicles [3], novel material design and characterization [4–6], Structural Health Monitoring [7, 8], robotics [9], civil and structural engineering [10, 11], etc. For example, in robotics, ML models play an essential role in providing the ability to sense and communicate with the world, make decisions, and learn from past experiences. In the field of structural health monitoring, ML methods are employed to monitor the safety and security of physical structures, including buildings, bridges, airplanes, and other electronic and mechanical equipment. With the help of these models, engineers can analyze data from vibration and strain measurements to identify structural faults and flaws, damage, and irregularities within the systems.

In the field of material modeling, the combination of ML and constitutive models is used to develop data-driven models that best represent complex, high-dimensional, and nonlinear material behaviors. These constitutive models that could be high-dimensional, history-dependent, or rate-dependent are used to estimate the mechanical behaviors of materials, such as stiffness, strength, ductility, failure, fracture toughness, and delamination [12] under various working conditions. It is also worth noting that ML techniques not only exhibit the feature of predicting material properties but also sometimes reduce computational time and costs by providing robust simulation and optimization tools for material design and processing [13, 14].

A successful data-driven ML-based material model should also replace classical phenomenological material models, which are commonly employed to study the behavior of materials in different forums. Phenomenological material models are usually based on the fundamental principles of physics obtained through empirical studies. These models are quite complex in an experiment, costly and time consuming in development, and sometimes do not provide a link between the microstructure details of the materials and the material design strategy. Thus, data-driven ML-based material models might overcome many of these challenges and complexities owing to their high-fidelity structures and dependence on a large and diverse dataset.

Furthermore, advanced engineered materials such as metamaterials have created new challenges and requirements for material modeling. These materials exhibit distinctive microstructure characteristics and demonstrate highly nonlinear behavior at the macroscale level owing to their complicated geometries and microstructures. Hence, there is an immediate need for highly robust models to evaluate data to identify patterns and trends that can be used to develop new or improve existing engineered materials with certain features and functionalities.

In recent years, a broad variety of material models have been designed based on machine learning (ML) or data-driven methods, which are promising methods for constitutive modeling of materials. For example, Pal and Naskar demonstrated that RF regression models could be useful to monitor several parameters and identify non-linear relationships between the properties of the elastomeric material [15]. Similarly, Liu et al. proved that support vector machine models are suitable methodology nonlinear and high-dimensional regression through small scale dataset as they help to eliminate local convergence issues [16]. As another example, Huang et al. have employed ANN models to train high-fidelity simulations and experimental data [17] in which the proposed framework was trained using displacement field data obtained from the experiments. They then observed and reported the limitations of the model over complex relations, such as viscoelasticity and plasticity, where the physical system is time-dependent. Hence, although ML-based constitutive modeling of materials has helped solve many problems with different perspectives to study the behavior of materials, there are still many challenges that need to be considered in this growing field of research.

This review paper aims to provide a pioneering comprehensive review as well as insights into the development of ML-based material models that are applied in simulations of various materials with a specific focus on material non-linearity, such as hyperelasticity, plasticity, visco-elasticity, and visco-plasticity. We then also investigate the ML-based approaches for modeling the structurally engineered materials which may present multiple novel functional properties. Furthermore, this review paper will provide the classification of ML-based models based on their appropriateness for the type of material non-linearity with focussing on theoretical and practical concepts of both machine learning models and physical material behaviors. Figure 1 presents an overview of the areas covered in this study including the data collection, analysis, and validation process. The first part of the figure presents the data collection processes for the design of the constitutive model of the material. Data might be obtained through experiments, simulations, or hybrid techniques, which are described in Section 2 of this review study. In addition to data collection, the performance of the constitutive models strongly depends on the selection of appropriate ML models. Thus, Section 3 presents ML-based material models appropriate for various material non-linearity and the classification of these methods based on their applications. The comparison of results and observations and opinions is addressed in Section 4. Finally, the study concludes with future research directions in Section 5.

## 2. Data generating processes

To develop a robust data-driven material model, it is crucial to generate high-fidelity and appropriate sets of data that can reflect all the physical phenomena of the investigated material. Various approaches and methods have recently been used by researchers to achieve reliable data, which could be from performing physical experiments, specific numerical simulations at various scales, and/or a combination of these two methodologies. These approaches, along with their challenges and benefits, are reviewed in this section to provide better directions for researchers on data generation for ML-based material modeling.

Classically, experimental methods were the first approach to investigate the physical behavior of the materials and to quantify these mechanical behaviors. There are several

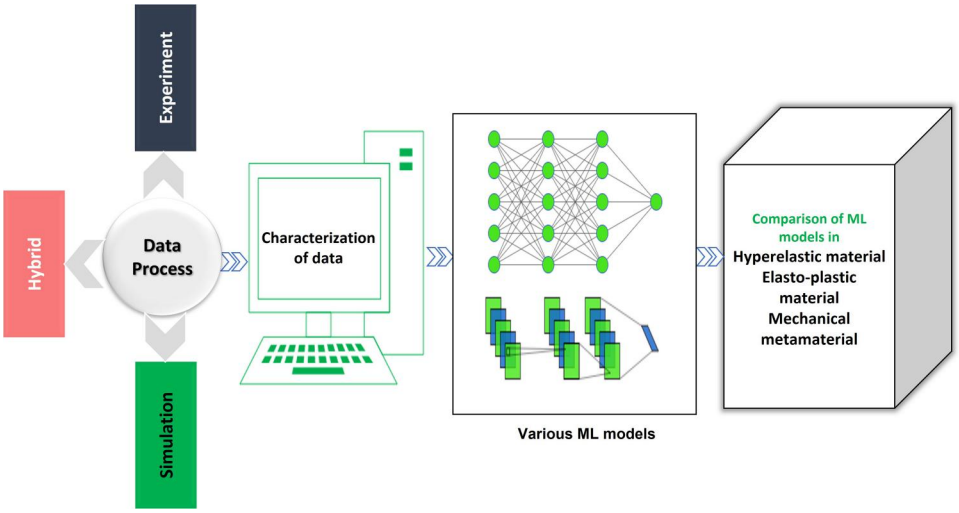


**Figure 1.** Overview of the data collection, analysis and validation process of an ML-based constitutive model.

different experimental methods that have been used to collect data for developing constitutive models for materials. For example, mechanical tests such as tensile, compression, biaxial, torsion, and bending tests can be performed to provide data on different material properties [18–21]. Zhou et al. [19] developed a method based on the transparent indentation method which was used to approximate the tensile deformation and stress of hyperelastic materials. Although the experimental indentation method has traditionally been used mostly for studying the mechanical properties of isotropic materials, they claimed that instantaneous mechanical properties exhibit anisotropic behavior during tensile deformation, resulting in an elliptical rather than a round contact zone.

We could summarize some of the advantages of these approaches as follows: (i) data and measurements from practical and real-world examples of mechanical materials, (ii) providing validation data for simulation-based models, (iii) developing actual data from different complicated small-size structures under various conditions, and (iv) developing a probabilistic dataset and considering uncertainties [22, 23] in the model based on repetition of experiments and, therefore, considering the measurement and laboratory errors in the nature of the models. However, experimental approaches have some significant limitations, such as (i) the limitation to generating a sufficiently large set of data, (ii) the limitation of obtaining all the required physical details or obtaining in-depth knowledge of the material, (iii) significant cost and time for conducting adequate experiments to obtain appropriate data, and (iv) challenges in interpreting the experimental data.

The second and most frequently used approach to collect data for data-driven material models is numerical simulations. Although these numerical simulations might be validated through some experiments, the simulations are the only data collection route for these researches. One of the most significant benefits of numerical simulations is its ability to generate enormous combined loading data sets, which can be challenging when performing experiments due to its limitations in terms of cost, time, and measurement equipment. For example, Fernandez et al. [24] used purely periodic boundary condition simulations on unit cell level to construct the constitutive behavior of a 3D cubic lattice using an ML-based approach. In the same concept, Chung et al. [25] used molecular dynamics (MD) simulation to develop a neural network constitutive model to study the hyperelastic behavior of polymers. The MD simulations in that study contained various loading such as uni-axial tension and compression, bi-axial tension and compression, tri-axial tension and compression, and simple shear. Furthermore, many studies employed the macroscale finite element method (FEM), as a straightforward and cost-effective way, to obtain an appropriate dataset for their non-linear ML-based constitutive models [26–29]. Among these numerical approaches, FEM is an appealing method for providing meaningful and relevant data to train ML algorithms with reasonable computational costs [30].

Considering the most important numerical approaches in the literature, we could observe that generating data through numerical simulations offers some advantages, as follows (i) it is more cost-effective in comparison to experimental methods, (ii) various complex design structures can be simulated under different loading conditions, (iii) some specific properties that cannot be measured through experiments can be captured in simulations, and (iv) it could be less time-consuming. However, these methods have some limitations such as (i) the models need to be verified and validated appropriately to generate trustworthy data, and (ii) implementation of high-fidelity material models, simulation strategies, and boundary conditions could be a challenge in numerical approaches.

Finally, the advantages and limitations of purely experimental and simulation approaches to obtain data for data-driven methods have led researchers to define a new framework that works more effectively and robustly than the first two approaches. This approach, which is the so-called "hybrid approach" in the community, combines the data collected from experiments and simulation analysis, maximizes the benefits, and reduces any potential drawbacks associated with individual processes. It is worth mentioning that this is a different methodology from using the experiments to validate the

simulations where all the final data comes from numerical analysis. However, in a hybrid approach, a specific percentage of the data is obtained from experiments, and the rest are derived from numerical analysis. Fahimi et al. [31] and then Narooei and Arman [32] used a hybrid approach in which they developed an objective function that was equal to the difference between the experimental results and those numerical simulation results to calculate the material parameters. Furthermore, Alawwa et al. [33] and Alkebsi et.al [34] used a combination of finite element simulation and experimental studies to perform full characterization of a novel lattice structure material to achieve enhanced mechanical performance under compression.

The advantages of the hybrid method include (i) combining experimental and simulation methods for more comprehensive results, (ii) capturing the detailed behavior of materials, and (iii) enhancing the accuracy and validation of the collected data. Moreover, certain limitations come with using hybrid approaches, such as (i) tending to be more complex and incorporating many other techniques as compared to experimental data and numerical simulations. Furthermore, it may be (ii) more expensive to implement a hybrid approach due to the additional resources, time, and expertise it needs [35].

## 3. Fundamental of ML approaches for material modeling

Researchers have recently developed ML as an efficient method for training algorithms incorporated with a data set of material properties. These ML algorithms identify complex relationships within datasets and predict behavior beyond the range of the initial data. The robustness of these material models is important for the material design process, material selection for a product, and prediction and avoidance of mechanical failures [36].

Kirchdoerfer and Ortiz [37] first introduced a data-driven material model that approximates the constitutive law directly from experimental materials data with relevant constraints and conservation laws and by circumventing traditional empirical modeling of materials. With such an approach, the empirical view of material modeling along with uncertainty and inaccuracy can be taken out without the loss of some experimental data. Later on, Eggersmann et al. [38] extended Kirchdoerfer and Ortiz model and introduced a model-free data-driven approach for inelasticity problems. Their study included the investigation of three different representations: (i) material with memory, which indicates that the dataset of the material has to depend on the material's previous history of deformation, (ii) differential materials, which refer to a material dataset with a short history of strain and stress, and (iii) the history variable, which indicates that the material dataset is dependent on ad-hoc variables that have a history of stress and strain information. They assumed that by using the material datasets of the differential material and history variable, they could represent the classical model of plasticity and viscoelasticity. Similarly, Conti et al. [39] extended the Kirchdoerfer and Ortiz work [37] to a finite-elasticity data-driven model. In their framework, they described the behavior of the material employing a material data set having all the states of the deformation gradient (F) and the first Piola-Kirchhoff stresses (P) in a constraint set that helps to keep its deviation from a material data set.

To implement ML-based material models, some essential steps have to be followed to obtain the complete benefits of ML and AI techniques. The step-by-step process to study the mechanical behavior of materials has been illustrated in Figure 2 and explained in detail in the following section. The first step is data generation, which can be done through either experimental analysis, simulation, numerical analysis, or a hybrid approach. This step has been explained in the previous section more comprehensively. The second step is the cleansing of data, which involves cleaning and sampling the acquired data to extract the desired features from the raw data and delete irrelevant information from the raw data. This will help reduce the complexity of the dataset while studying high-dimensional or 3D problems of advanced materials. In the third step, the appropriate ML approach is selected based on the type of data, physics, and nature of the problem. This may be a regression, classification, or clustering problem. In this regard, the majority of the ML-based models that are developed to study the constitutive behavior of materials are the tensor basis neural network (TBNN), symmetric positive definite neural network (SPD-NN) [40], feedforward neural network (FFNN)[24], equilibrium basis convolution neural network (ECNN) [41], deep material network (DMN) [42], artificial neural network (ANN) [43, 44], constitutive artificial neural network (CANN) [45], deep energy method (DEM)[46], and etc. The theoretical background of these methods has been discussed in detail in the following. Based on the selection of the ML approach, the next step is to train the model with the processed data characterized in the second step. The data set is classified as training data, testing data, and sometimes cross-validation data, which should be separated to avoid overfitting during the training of the model. Finally, every ML-based model requires an evaluation step to ensure accurate prediction and performance regarding the behavior of materials. Parameters such as mean square error (MSE), root mean square error (RMSE), training and validation losses, and stress-strain predictions are examples of parameters to be considered during the evaluation process of an ML-based model.

To better understand the process of choosing an ML approach for a material model, we first need to understand the theoretical background of each ML methodology and their mathematical specifications. For example, the random forest algorithm is fundamentally made up of decision trees, as schematically illustrated in Figure 3a. In constitutive materials modeling, decision trees capture the relationship between input and output parameters by partitioning the features to predict the behavior of the complex material. Moreover, RF usually combines many classification trees based on ensemble learning principles, with the prediction connection being randomly updated throughout implementation to increase the diversity of the forest's types of trees [47, 48]. Since RF relies on feedback from each decision tree

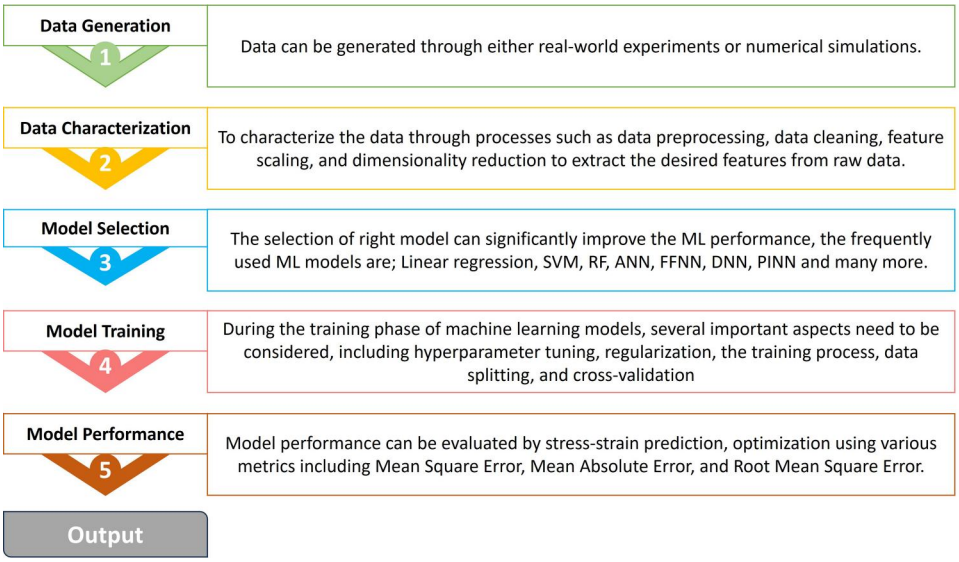


**Figure 2.** The step-by-step development process of validated ML-based material models.

to determine the ultimate output, it usually takes longer time to make the decisions and therefore, it is complicated to make a fast framework based on RF. It is also important to discuss that Bootstrap is a critical technique for RF where a new training dataset is made by repeatedly generating new sample data randomly from the original training data. For example, Liu et al. [49] have used RF together with the Bootstrap approach to generate prediction trees for a lattice-structured material which generate a functional relationship between four lattice features (X) and the equivalent elastic modulus of the lattice structure (Y) as

$$\mathrm{Y} = \frac{1}{n}\sum_{i=1}^{n} \mathrm{Y}_i = \frac{1}{n}\sum_{i=1}^{n} \mathrm{f}(\mathrm{X}, \mathrm{T}_m^i) \tag{1}$$

where n, is the number of prediction trees, $\mathrm{T}_m = (\mathrm{X}_1, \mathrm{Y}_1), (\mathrm{X}_2, \mathrm{Y}_2), \ldots, (\mathrm{X}_m, \mathrm{Y}_m)$ is the training set. Such an approach helps to introduce randomness and diversity into the training process, reducing over-fitting and improving model convergence with the final output.

Among the other ML approaches, ANN stands out as one of the widely used ML models for tasks such as regression, classification, prediction, pattern, and image recognition, while SVM is popular for detection, classification, and regression in designing constitutive materials modeling. The key differences between ANN and SVM lie in terms of the representation and pattern recognition approach. As presented schematically in Figure 3b and c, SVMs aim to find a hyperplane or decision boundary to separate classes in the input space, while ANNs map inputs to outputs through transformations and activations in hidden layers, producing continuous or discrete output values. Furthermore, SVMs find a hyperplane in the input space to separate patterns, utilizing a kernel function for non-linearly separable data, while ANNs, especially deep neural networks, learn complex non-linear mappings by composing multiple layers of neurons applying non-linear transformations to the input values [50, 51].

Furthermore, CNN, as illustrated schematically in Figure 3e, is one of the types of deep neural networks that are well suited to processing spatially structured data using weight-sharing and pooling layers for various regions of images and volumes. These networks show great potential to determine the complex relationship between strain distributions and elasticity parameter fields by accurately obeying fundamental physical equations [52]. Furthermore, the development of RNN models, presented in Figure 3d, plays a significant role in advancing data-driven modeling for elastic-plastic and viscoelastic materials mainly due to the ability to incorporate time and history dependence. Further fundamental theoretical concepts of such models are explained in the elastoplastic and viscoelastic sections of the paper.

The Physics-Informed Neural Network (PINN), as illustrated schematically in Figure 3f is another branch of ML-based methods that work effectively for material modeling. This method integrates fundamental physical laws and engineering design knowledge with the neural network training process. The purpose of this integration is to boost the performance of the model by solving various problems with better accuracy and improving the generalizability of the material model and as a results it has been growing significantly in computational mechanics forum in the recent years. For example, the PINN approach has been used successfully for the prediction of structural instability of materials [53], the prediction of multiaxial fatigue life [54], structural optimization [55], and inverse engineering structural problems [56]. Furthermore, the PINN models have the ability to be trained with a small amount of data therefore, it could improve the computational cost and training efficiency [57], interpretability, and prediction accuracy. The critical aspect of PINN, which plays a fundamental role in ensuring accurate learning of the model and is shown in Figure 3f, is the total cost or loss function as a representation of both the observed data and the underlying physics of the problem. It provides direction for the training procedure and facilitates the obtaining of solutions efficiently and practically in the scope.

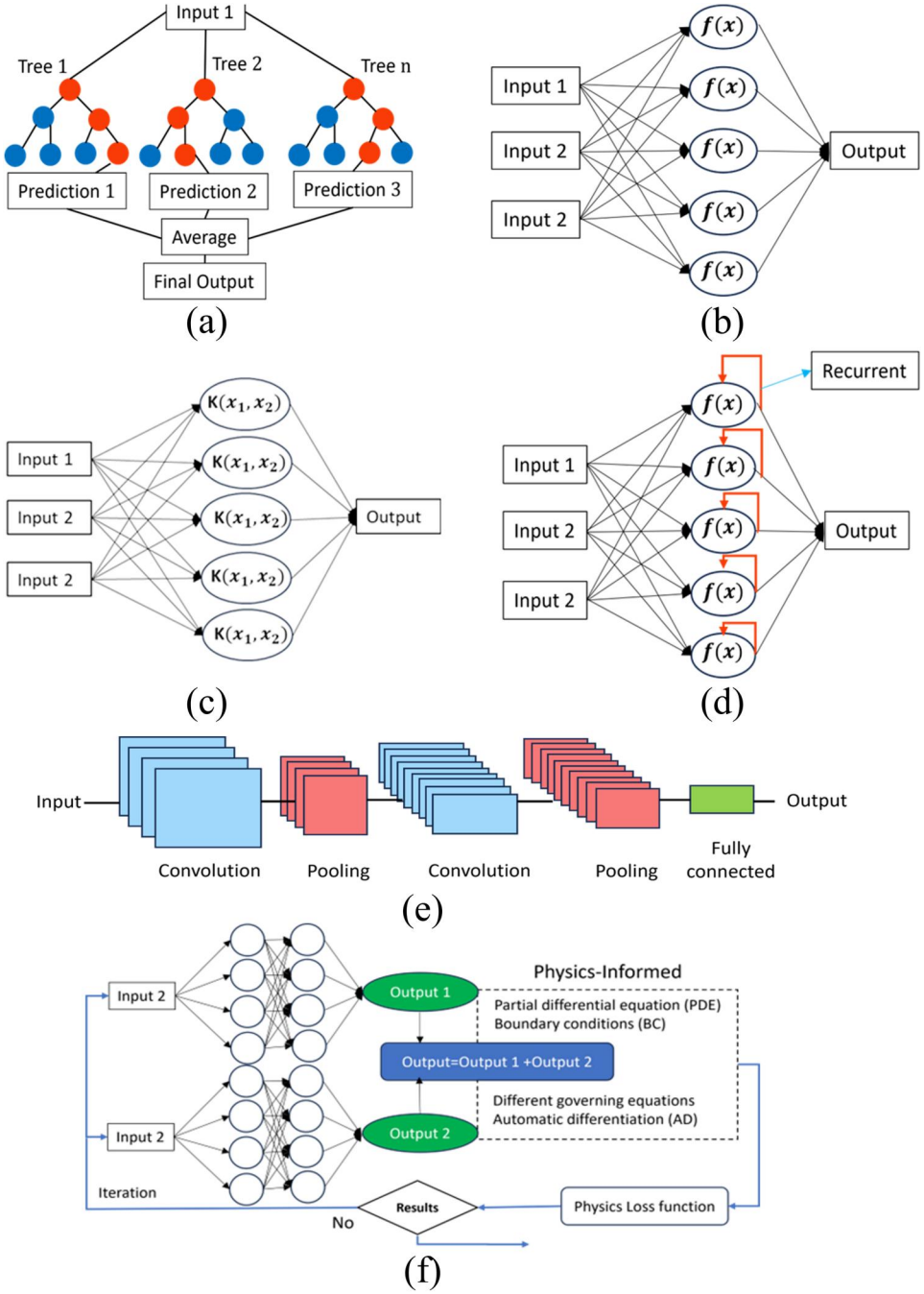


**Figure 3.** The schematics of various ML-based models for constitutive modeling of materials.

In summary, these various ML-based methods provide important insights regarding their potential benefits and limitations in constitutive modeling of materials. We could clearly observe here that examining inherent elastic materials typically does not require sophisticated ML models unless there are unique motivations for their utilization. Therefore, regression- or classification-based ML models are commonly used for elastic materials[58, 59]. However, in other cases, more complex behaviors, such as non-linear material responses, anisotropic characteristics, or material behaviors under extreme conditions, must be captured which require more sophisticated and advanced models. Therefore, in the following sections, we focus and review the implementation of ML-based models for various non-linearity in material behaviors.

## 4. ML-based approaches for material non-linearity

There is a reasonable discussion in the scientific forum that we don't need any data-driven model when the physical material behavior is very simple and involves only a few material constants such as isotropic linear elasticity and what would be the gain of adding extra modeling complexity?

While this is a true statement that ML-based methods would add complexity to simple physical material models such as linear elasticity, we should not ignore the fact that ML-based models could be fantastic tools for linear regressions for anisotropic linear elastic materials where phenomenological models started to become more sophisticated. Furthermore, another advantage of Ml-based models is the capability of offering probabilistic approaches that could

consider the uncertainty and variations in experimental data from material characterizations.

Considering all the rapid advances in the field of ML-based material models as well as considering the fact that a model that covers nonlinearity in material models could usually be used for linear elasticity, we focus our study on application of ML-based models for nonlinear material behaviors. To this aim, in this section we will focus on hyper-elasticity, visco-elasticity, viscoplasticity, and the combined behavior in structural engineered materials.

### 4.1. ML-based models for nonlinear elasticity (hyperelasticity)

Hyperelastic materials are a type of material which can endure large deformation before failing and still remain elastic. This means that the deformation is fully reversible with no plastic deformation when the load is removed. This also indicates that the stress-strain relationship of hyperelastic materials is highly nonlinear. The principle of strain energy density serves as the theoretical basis of constitutive modeling of hyperelastic materials. This energy density is a function of the deformation of the material and could be used to determine the stress-strain relationship through constitutive tensor. Therefore, all classical constitutive models for hyperelsatic materials present a type of phenomenological model for the strain energy function that includes various material constants. These material constants would be identified by fitting the model to the experimental data. Some famous theoretical hyperelastic models include but are not limited shown in Table 1.where $I_1$, $I_2$, and $I_3$ are three invariants of strain tensor as

$$\begin{aligned} I_1(\mathbf{C}) &= tr(\mathbf{C}) = I_1(\mathbf{B}) \\ I_2(\mathbf{C}) &= \frac{1}{2}\left[tr^2(\mathbf{C}) - tr(\mathbf{C}^2)\right] = I_2(\mathbf{B}) \\ I_3(\mathbf{C}) &= det(\mathbf{C}) = I_3(\mathbf{B}) \end{aligned} \tag{2}$$

with $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ and $\mathbf{B} = \mathbf{F}\mathbf{f}^t$ are right and left Cauchy-Green tensors, respectively, and $\mathbf{F}$ is the deformation gradient. The stress tensor and elasticity tensor would then be found by using the first and second derivative of the strain energy function with respect to the right Cauchy-Green deformation tensor, respectively as

$$\begin{aligned} \mathbf{S} &= 2\frac{\partial W}{\partial \mathbf{C}} \\ \mathbb{C} &= 2\frac{\partial \mathbf{S}}{\partial \mathbf{C}} = 4\frac{\partial^2 W}{\partial \mathbf{C}^2} \end{aligned} \tag{3}$$

where $\mathbf{S}$ is the second Piola-Kirchhoff stress tensor and $\mathbb{C}$ the fourth-order elasticity tensor, respectively.

Therefore, considering the importance of data in finding material parameters for traditional hyperelastic models, researchers started to discuss data-driven approaches to directly find the constitutive model from data without involving phenomenological consideration. There were various approaches for this purpose in the literature, such as training a data-driven model to represent the strain energy function or developing a model to directly link large deformation stress components into the stress tensor, which will be discussed in this section. These ML data-driven approaches have significant advantages over phenomenological models which include but are not limited to the absence of phenomenological assumptions, the independence of parameter calibration and the adaptation of the iterative model using new data [60, 61].

Several ML-based models are designed to learn the strain energy density from synthetic and experimental data for hyperelastic materials. Pal et al. [15] developed three different regression ML models, including linear regression, support vector regression (SVR), and random forest (RF), to determine the effectiveness of the ML model in developing a model for Marlow hyperelastic material. They collected the data through an experimental process on rubber with 10 samples analyzed for every test. According to their outcomes, the linear regression model could not accurately predict the performance parameters such as mean square error (MSE) and mean absolute error (MAE). Furthermore, the linear regression model produced outcomes with some degree of randomness when compared to results from SVR. However, the RF regression model consistently produced the most reliable and deterministic outputs when compared to the other three models.

The other hyperelastic material model based on a NN was presented by Shen et al. in [62]. Their model has been trained by employing the test data from rubber that could approximate the hyperelastic strain energy function. The inputs of NN are two strain invariants along with the volumetric strain ratio J and the trained model predicts the strain energy. Although the ML model trained well to show better performance as compared to existing strain energy functions, some practical considerations should be taken into account while gathering test data for rubber material in order to train the neural network. In [45], they introduced a constitutive ANN model for hyperelastic materials that could include data from three different ways, i.e. stress-strain, theoretical knowledge from the field of material theory, and also supplementary knowledge such as knowledge of microstructure or materials processing. Such an ML

**Table 1.** Summary of the some key phenomenological hyperelastic models.

| Model name | Strain energy funcion | Material parameters | Description |
|---|---|---|---|
| Neo-Hookean | $W = C_{10}(I_1 - 3)$ | Only one parameter $C_{10}$ | A basic model suitable for small strains |
| Mooney-Rivlin | $W = C_{10}(I_1 - 3) + C_{01}(I_2 - 3)$ | two parameters $C_{10}$ and $C_{01}$ | Suitable for moderate deformations under 200% |
| Yeoh | $W = \sum_{i=1}^{3} C_{i0}(I_1 - 3)^i$ | three parameters $C_{10}$, $C_{20}$, and $C_{30}$ | Employing for rubber-like materials and capturing material behavior using multiple parameters |
| Ogden | $W = \sum_{i=1}^{N} \frac{\mu_i}{\alpha_i}(\lambda_1^{\alpha_i} + \lambda_2^{\alpha_i} + \lambda_3^{\alpha_i} - 3)$ | N (user-defined) parameters $\mu_i$ and $\alpha_i$ | Suitable for wide strain range and better flexibility than the Mooney-Rivlin model in describing curves |
| Gent | $W = \frac{E}{6}(I_m - 3)ln\left(1 - \frac{I_1 - 3}{I_m - 3}\right)$ | Two parameters $E$ and $I_m$ | Robust, mathematical simple and easily combined with physical basis and suitable for large deformation |

model would help reduce the required datasets for training by including continuum mechanical knowledge. As a result, the method would theoretically be able to predict the characteristics of new hyperelastic materials using knowledge passed over direct mechanical or geometrical explanation.

Moreover, Li and Chen [41] proposed an equilibrium-based convolution neural network (ECNN) constitutive modeling of hyperelastic material which is used to employ displacement, strain and applied external force as input information to train the model while stress is considered as an internal variable. They found that enormous training data could be obtained using a single specimen that deforms unevenly under loading, and it was concluded that these techniques are a substantial source of data generation. However, stress related to a certain collection of strains could be achieved by implementing equilibrium equation intrinsic requirements within this proposed model. All strain measurements in this study are based on logarithmic strain, and the resulting deformation dataset includes 16,848 distinct datasets. An unsupervised convolution neural network was then designed to isolate the spatial stress components in irregular deformation. The high level of consistency suggests that the designed ECNN is capable of accurately representing the local stress within the non-uniformly deformed material. The proposed model is presented only for 2D problems however, they claimed that their design could be extended to solve 3D problems by using volumetric digital image correlation (V-DIC) that helps to measure the internal body deformation. Furthermore, the model only contemplated history-independent hyperelastic constitutive behavior, and for materials with history-dependent properties such as viscoelastic or viscoplastic materials other types of the model should be developed.

Physics-informed neural networks (PINN) models could also be employed to identify the constitutive relationships of hyperelastic materials. These models provide versatility in investigating hyperelastic material properties, encompassing applications such as resolving inverse problems, implementing multiscale modeling, establishing constitutive models for hyperelastic soft tissues, and studying hyperelastic foams and composites with remarkable precision and reliability. Moreover, PINN incorporates potential energy, the collocation method, and deep learning to identify the partial differential equations (PDE) that determine the mechanical deformation of hyperelastic materials. The implementation of PINN to address PDEs is a more promising approach, however, it comes with its own set of challenges and complexities. For example, the weight and biases of the PINN models are generally nonconvexly identified by using the optimization problem and the automated differentiation (AD) utilized for measuring spatial gradients is unstable [63]. The standard PINN models are usually unable to accomplish appropriate outcomes when addressing hypoelastic materials challenges, mainly due to the significant deformation experienced by hyperelastic materials. In order to address such challenges, Luo et al. [64] proposed stepwise PINN (sPINN) (a combination of PINN and Hughes-Winget algorithm) to solve large deformation-related problems in hypoelastic materials. The model is trained with different numerical synthesis datasets having different training points including 700, 1000, and 1500. The results indicated that the sPINN exhibits the ability to effectively and accurately predict the displacement and stress distributions in path-dependent large deformation scenarios on small datasets. Despite this, the concentration factor is challenging for sPINN to capture precisely and the entire training procedure requires a considerable amount of time.

Finally, to better summerize and classify the suitable ML-based approaches for hyperelasticity, we have provided Table 2 as a comprehensive summary of different ML models for hyperelastic material including their limitations and advantages.

### 4.2. ML-based models for plasticity and visco-plasticity

Elastoplastic materials demonstrate unique properties due to the combination of elastic and plastic properties, yield stress, ultimate stress, and strain-hardening qualities. In addition, it offers the property of hysteresis when subjected to cyclic loads. Hence, to understand and design these materials, it is crucial to develop high-fidelity material models that capture their complex properties. The general stress-strain relations of a typical elastoplastic material is the combination of the elastic part $\boldsymbol{\varepsilon}_{\mathbf{e}}$ and plastic part $\boldsymbol{\varepsilon}_{\mathbf{p}}$ as

$$\boldsymbol{\sigma} = \mathbb{C} \cdot (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_{\mathbf{p}}) \tag{4}$$

where $\mathbb{C}$ is the fourth-order elastic tensor and $\boldsymbol{\varepsilon}$ is the total strain having an elastic part and a plastic part. Therefore, the main part of developing an elastoplastic constitutive equation is the development of the phenomenological model for plastic strain, $\boldsymbol{\varepsilon}_{\mathbf{p}}$. This usually includes the material constants that need to be determined after fitting the model into experimental data. However, this is a challenging step in phenomenological elastoplastic material models as it might not be possible to perfectly fit the model to experimental data through moderation of material constants.

To address this for elastoplastic materials, data-driven models based on ML are designed to accelerate the development of the model by predicting $\boldsymbol{\varepsilon}_{\mathbf{p}}$ based on training over history data [92]. Since plastic flow depends not only on the current stress level but also on the loading history, to develop a plastic material model, the fundamental data set should be based on the stress-strain relationship and also the stress-strain sequence pairs. Hence, training a data-driven plasticity model requires sequence data from many loading-unloading paths, knowing that every strain-stress sequence pair represents a single loading-unloading path. For example, equation 5 represent a typical ML-based elastoplastic material model

$$\boldsymbol{\sigma}^t = f^{ML}(\boldsymbol{\varepsilon}^t, \mathrm{h}^t) \tag{5}$$

where $\mathrm{h}^t$ represents loading history, $\boldsymbol{\sigma}^t$ and $\boldsymbol{\varepsilon}^t$ are total stress and strain at time $t$ obtained from the experiment, respectively, and $f^{ML}$ is a trained ML-based function.

Among various ML approaches which are discussed in the previous sections, ANN is an appropriate method for analysis of elastic strain part of an elastoplastic strain

**Table 2.** A summary of important ML-based models for hyperelastic behavior.

| ML models | Limitations | Advantages | References |
|---|---|---|---|
| ANN | Inconsistent convergence rate and model performance susceptible to the selection of optimal parameters | Mapping non-smooth function and high dimensional multiple input-output with improved model accuracy | [40, 65–69] |
| FFNN | Interpretability risk and requires a huge dataset of labeled data for several models | offers universal function approximation, simple to implement and can act as a convex function. | [50, 70–74] |
| Physics-informed NN (PINN) | Challenges include formulation and computational cost | Exhibits strong extrapolation ability, fast convergence, high accuracy and satisfies polyconvexity | [75–82] |
| CNN | limited to grid inputs and struggle with unstructured input meshes | Provide better generalization, high computational efficiency, and support interpretability | [41, 83–87] |
| SVM | Computational complexity for large-scale datasets, limited scalability, and limited interpretability | Performs well in high-dimension space, has better generation ability, accuracy and also provides convex loss function | [88–91] |

function which is due to the relatively straightforward nature of elastic strain. However, for the plastic strain part which depends on history data of strain, the RNN approach would be more suitable. This could be explained through the theoretical background of RNN which is made from hidden layer neurons that have connections with looping or cyclic topology. As explained mathematically in [93], the RNN architecture enables the hidden layer output $\mathbf{H}^t$ to be influenced by the previous input $\mathbf{x}^t$ at the time step $t$ as well as the hidden output itself at step $(t-1)$ allowing the network to have room for time-dependent relationships. These characteristics of the RNN could be represented mathematically as

$$\mathbf{H}^t = f\left(\mathbf{W}_1\mathbf{x}^t + \mathbf{U}\mathbf{H}^{t-1} + \mathbf{b}_1\right) \tag{6}$$

where, $f$ is the activation function, $\mathbf{W}_1$ is the weight, $\mathbf{b}_1$ is bias for the hidden layers, and $\mathbf{U}$ is the matrix representing the recurrent connection between the hidden layer at subsequent steps. Therefore, $\mathbf{U}\mathbf{H}^{t-1}$ component is the extra element that RNN models have in comparison to a standard ANN which incorporates the sequential data into the model. Following the same concept, Heider et al. [94] employed a hybrid neural network that combined the traditional feed-forward neural network with an RNN to handle path-dependent material responses. The integrated supervised ML model is trained with a dataset of 1176 experiment samples. Due to the limitation of interpretability of standard deep neural network predictions, they developed intermediate predictions that attempt to comprehend stress-predicting mechanisms by adding the concept of graph theory. Graph theory is implemented to design models for large-scale, high-fidelity solutions to continuum physics challenges. Similarly, Wang et al. [95] designed a model to generate data for history-dependent constitutive responses using a multi-agent meta-modeling strategy. The multi-agent meta-modeling strategy involves two main components, the model agent works to predict the output stress from the input strain history and data agents collect data from molecular dynamics and discrete element simulations with the help of the modeler agent in order to improve the quality of predictions by employing reinforcement supervised learning technique.

Although, RNNs have the benefit of retaining information from previous computations, allowing them to capture sequential relationships in the data, they are sensitive to vanishing gradients, which may limit the training process. To circumvent this limitation, the concept of Long-Short Term Memory (LSTM) was developed. The LSTM model is presented in [96] for the accelerated elastoplastic analysis of heterogeneous materials. It consists of a memory cell or current cell, $\mathbf{C}_t$, and three gate layers so-called forget gate, $\mathbf{f}_t$, input gate, $\mathbf{i}_t$, and the output gate, $\mathbf{o}_t$ as

$$\mathbf{C}_t = \mathbf{f}_t \odot \mathbf{C}_{t-1} + \mathbf{i}_t \odot \bar{\mathbf{C}}_t \tag{7}$$

with

$$\mathbf{f}_t = \sigma\left(\mathbf{W}_f^h \cdot \mathbf{h}_{t-1} + \mathbf{W}_f^x \cdot \mathbf{x}_t + \mathbf{b}_f\right) \tag{8}$$

and

$$\mathbf{i}_t = \sigma\left(\mathbf{W}_i^h \cdot \mathbf{h}_{t-1} + \mathbf{W}_i^x \cdot \mathbf{x}_t + \mathbf{b}_i\right) \tag{9}$$

where $\mathbf{W}_f^h$, $\mathbf{W}_f^x$, $\mathbf{b}_f$ are the weights and bias of the forget gate layer, $\mathbf{W}_i^h$, $\mathbf{W}_i^x$, $\mathbf{b}_i$ are the weights and biases of the input gate layer, $\sigma$ is the activation function, and $\mathbf{x}_t$ is the current input. The new information then could be added by using a temporary cell state $\bar{\mathbf{C}}_t$ which combines data from the previous hidden state and the current input as

$$\bar{\mathbf{C}}_t = \tanh\left(\mathbf{W}_c^h \cdot \mathbf{h}_{t-1} + \mathbf{W}_c^x \cdot \mathbf{x}_t + \mathbf{b}_c\right) \tag{10}$$

where $\mathbf{W}_c^h$, $\mathbf{W}_c^x$, $\mathbf{b}_c$ are the weights and bias of the temporary cell state with the tanh activation function. Thus, the hidden state $\mathbf{h}_t$ can be updated through the output gate layer as

$$\mathbf{h}_t = \mathbf{o}_t \odot \tanh(\mathbf{C}_t) \tag{11}$$

where

$$\mathbf{o}_t = \sigma\left(\mathbf{W}_o^h \cdot \mathbf{h}_{t-1} + \mathbf{W}_o^x \cdot \mathbf{x}_t + \mathbf{b}_o\right) \tag{12}$$

and $\mathbf{W}_o^h$, $\mathbf{W}_o^x$, $\mathbf{b}_o$ are the weights and bias of the output gate layer.

Table 3 provides a perspective summery on the range of ML models used in elastic-plastic and visco-plastic constitutive models, including their limitations and advantages. As can be seen in Table 3, there has been a significant shift in the primary approach to designing ML-based models for plasticity over the years as new developments and insights have emerged. Although initially ANN and SVM models were employed for plasticity behavior, the most recent research is focused on the development of RNN, GANN, and PINN models. This is specially related to their unique ability to leverage history-related aspects of materials.

Table 3. A summary of important ML-based models for plasticity and visco-plasticity behavior.

| ML models | Limitations | Advantages | References |
|---|---|---|---|
| RNN | Vanishing and exploding gradients are common challenges and can be avoided using LSTM and GRU | Ability to leverage sequential data and history-dependent constitutive modeling | [97–105] |
| ANN | Overfitting and required large datasets and loss of accuracy for over-complex models | Overall computational efficiency and easy implementation | [106–111] |
| PINN | Complex implementation, formulation and also required a comprehensive understanding of physics laws (nonlinear hardening and softening law) | Improving the stability, data efficiency, extrapolation, and representing complex behaviors | [112–115] |
| SVM | performance highly depend on the choice of kernel function that needs a deep understanding within the domain knowledge | Effective for high-dimensional space, and computational efficiency | [116–118] |
| Generative Adversarial Networks (GAN) | To generate better realistic samples, GANs need to incorporate physical knowledge which can be computationally intensive | Generate high-quality synthetic data of the arbitrary size of the material parameters, and also the ability to extrapolate beyond the training range and improve training efficiency | [119–121] |

### 4.3. ML-based models for visco-elasticity

The Visco-elastic behavior is a result of the internal structure of some materials, which typically consist of complex, interconnected polymer chain structures. The modeling of viscoelastic materials obtains its theoretical foundations from principles in physics and mechanics that include time-dependent constitutive models, energy dissipation, Rheological models, temperature and frequency influences, etc [122, 123]. The theoretical background of the viscoelastic model originated with the incorporation of viscoelastic behavior with the help of the Kelvin-Voigt model into the initial fundamental model proposed by Winkler [124]. This spring-damper-based model could be recapped as

$$P(x,t) = kw(x,t) + c\dot{w}(x,t) \tag{13}$$

where $kw(x,t)$ and $c\dot{w}(x,t)$ represent the linear elastic and viscoelastic behaviors, respectively, with $k$ is stiffness, $c$ is a damping factor, $w(x,t)$ and $\dot{w}(x,t)$ are displacement and velocity, respectively. This equation is generally employed in developing a classical constitutive model for viscoelastic materials, where both elastic and viscous components contribute to the overall behavior. Later, Winkler's original model is improved by many other models such as Maxwell, Zener, Poynting-Thomson, Burger Filonenko-Borodich, Hetenyi, Pasternak, Kerr (three-parameters), Half-space, Vlasov, and Reissner [122].

Consequently, ML-based data-driven constitutive models provide outstanding capabilities for analyzing the complex properties and behaviors of viscoelastic materials by replacing the sophisticated physical theorems and phenomenological models with material models that are driven directly from data. These models are trained on large datasets of numerical and experimental data to learn the complex relationships between various factors that influence the behavior of viscoelastic materials like stress-strain, temperature, time, and various loading conditions. Prusty et al. [125] proposed an inverse identification method based on a neural network optimization (NNO) algorithm that identifies the frequency-dependent constitutive parameters of viscoelastic materials that were then experimentally verified. Viscoelastic materials exhibit frequency-dependent features in their constitutive parameters, particularly the storage and loss modulus, which makes studying these properties critical for a comprehensive understanding of viscoelastic materials. The NNO method accurately predicted the constitutive parameters and demonstrated excellent agreement with the experimental results. The theoretical concept of NNO is based on the gradient-based interior-point algorithm (IPA) which is used to solve optimization challenges.

As discussed earlier, RNN models have the capacity to capture long-term time dependency in the data. Therefore, not only are they a good ML-based approach for elastoplastic materials but also are an ideal option for modeling viscoelastic materials. Chen has developed an RNN model to represent the viscoelasticity in 1D and 3D cases [126]. The numerical algorithm for viscoelastic modeling comprises the implementation of the generalized Maxwell material model as

$$\boldsymbol{\sigma}_{n+1} = U^{0'}(\Theta_{n+1})\mathbf{1} + \gamma_{\infty}\mathbf{S}^{0}_{n+1} + \sum_{I=1}^{N}\gamma_I \mathbf{h}^{(I)}_{n+1} \tag{14}$$

where $U^{0'}(\Theta_{n+1})\mathbf{1}$ and $\mathbf{S}^{0}_{n+1}$ represent the initial bulk stress tensor and the initial elastic deviatoric stress tensor at time $t(n+1)$, respectively, and $\mathbf{h}^{(I)}_{n+1}$ is the transient deviatoric stress tensor in the $I-th$ Maxwell element at the time $t(n+1)$. Furthermore, $\gamma_I = \frac{\mu_I}{\mu}$ represents the fraction of elastic shear modulus at $I-th$ Maxwell element to the total shear modulus $\mu = \mu_{\infty} + + \sum_{I=1}^{N}\mu_I$. This developed RNN model is also capable of predicting the viscoelastic behavior beyond the test data by utilizing extrapolation. The model's performance across the training and validation datasets is consistent, suggesting the design of a stable and resilient model.

Similar to RNN models, PINNs have acquired popularity for analyzing the complex behavior of viscoelastic materials. PINNs stand out for their ability to integrate ML with fundamental physics principles, making them the method of choice for investigating the unique behavior of viscoelastic materials. Dabiri et al. [127] developed neural networks that take into account insights from multiple fractional constitutive models. The developed fractional rheology-informed neural networks (RhINNs) are then used to identify the relevant parameters for three fractional viscoelastic constitutive models including the Maxwell, Kelvin-Voigt and Zener models. The output of the model in [127] is a material response which is $\sigma(t)$ for the fractional Maxwell model and the fractional Zener model and $\epsilon(t)$ for the fractional Kelvin-Voigt model. Hence, this approach proposes a robust framework for the data-driven inverse solution of fractional constitutive models, aiming to enhance the effectiveness of the solution process. Another important mechanics-informed data-driven method was developed in [128] to train the

model from the constitutive law of nonlinear viscoelastic material with stress-strain data. What makes these models important is that these types of mechanics or physics-informed models not only provide stable and high-precision models but also efficiently incorporate mechanics-based constraints into the model's architecture and loss function, such as dynamic stability, material stability, objectivity, internal variable stability, and consistency.

In general, ML models are an effective technique for investigating the complex properties of viscoelastic materials. However, the nature of the problem and the features of the data set should influence the choice of an ML model. For example, in [129] three ML models including SVM, relevance vector machine (RVM), and RF are employed to predict the dynamic viscoelastic properties of asphalt binders. The dataset for dynamic viscoelastic properties has 10 macroscale distinct parameters, whereas the dataset for composition parameters contains 29 microscale distinct parameters used for all these models. Even though the dataset was small, the SVM outperformed the other two models in terms of efficiency and accuracy in modeling viscoelastic properties. This is due to the Gaussian function being chosen as the SVM kernel function, resulting in impressive performance under general smoothness assumptions. Similarly, six ML models such as ANN, Robust Linear Regression, Linear SVM, Decision Tree Regression, Gaussian Process Regression (GPR) and Ensemble Regression are used in [130] to predict the viscoelastic behavior of modified bitumen. In relation to the linear nature of the data, most linear ML models succeeded in making accurate predictions. However, in terms of error metrics, Ensemble Regression proved to be the most effective method for predicting the viscoelastic properties of modified bitumens. In contrast, ANN and GPR demonstrated the best performance of the correlation metric. Therefore, the selection of an appropriate ML-based model for viscoelasticity depends on the specific task and the characteristics of the data.

In Table 4, various ML approaches which are appropriate for developing constitutive models for viscoelastic materials are summarized comprehensively. The table systematically outlines the key information on the data types used, dataset sizes, model types employed, and the efficacy and robustness of the models in making predictions. The primary observation is that RNN models are considered the preferred choices for viscoelastic material modeling because of the ability to account for history and time dependence in the material behavior. Furthermore, it is noteworthy that certain ML models are integrating the LSTM concept to account for and incorporate the history and time-dependent behavior of viscoelastic materials.

### 4.4. ML-based models for non-linear architectured materials

In recent years, there has been an increase in the development of architectured materials with multi-functional features that illustrates several non-linear material behaviousr [145–150]. Therefore, for effective simulations of macroscopic structures and to optimize the nonlinear mechanical behavior associated with the fundamental unit cells of such architectured materials, a high-fidelity and robust material model is essential. Challapalli et al. have recently described a new design optimization method that uses statistical analysis techniques and supervised ML regression models with a dataset of 2000 fingerprint samples to study mechanical metamaterial [151]. The objective of their research was to develop and design thin-walled cellular structures with highly increased strength and recovery stress. They claimed that no prior integration of these methods for structural optimization has been provided, even though the single models used in this study have been widely used in other research investigations. For example, they used ML regression models and generated adversarial networks (GAN) to optimize 3D lattice unit cells for uniaxial and multiaxial strengths in their previous work [152]. They also introduced the very first approach that uses inverse ML with high-performance architectures that find, evaluate, and optimize particular lattice unit cell designs. The GAN provides numerous possible lattice unit cells for the inverse design framework incorporated into the forward regression model. The obtained lattice structures were determined to have a greater load-sustaining capacity than that of the octet lattice structure. Although the developed inverse ML model can extensively be utilized for many other purposes, it works exceptionally well in optimizing additional load-bearing metamaterial structures.

**Table 4.** A summary of important ML-based models for viscoelastic materials.

| ML models | Limitations | Advantages | References |
|---|---|---|---|
| RNN | • large data requirements,<br>• computational cost specially when using LSTM and GRU,<br>• the dimensionality of the problems affects the extrapolation ability. | • Sequential data handling and longer time sequence,<br>• Handling dynamic relationships (memory of previous states and nonlinear) | [126, 131–135] |
| K-means Clustering | • Too high dimensions may affect the accuracy and efficiency,<br>• Sensitive to the initialization of the clusters. | • Easy to implement,<br>• Adapt to various shapes and sizes of clusters for different data | [136, 137] |
| PINN | • Complexity in formulating cost functions,<br>• High computational cost | • Reduce data dependency and capture rate-dependency,<br>• Improved generalization and extrapolation,<br>• Can include and study complex phenomena | [128, 138–141] |
| SVM | • High-dimensional spaces with non-linear kernels) can be challenging,<br>• necessity of pre-processing the data through normalization | • Robustness to Overfitting<br>• Carrying out risk minimization from the loss function. | [129, 142–144] |

Xue et al. [153] have extended the NN-based method for modeling the response of non-linear elastic material for small strain cases which was initially presented in [154] to simulate the non-linear mechanical behavior of cellular architectured materials subjected to large deformations. To achieve this goal, they acquired training data through a significant number of represented volume element (RVE) simulations at the microscopic or cellular level. Based on these data, they trained an NN model to represent the macroscale effective strain energy density, a function of macroscopic strain and microscopic structural properties. Although their NN model is a viable alternative to costly FEA for designing and analyzing architectured materials, this work is limited to 2D applications and does not include material symmetry in the model explanation. Furthermore, Xie et al. have implemented an AI algorithm based on ANN to solve the transient bending properties of a metamaterial by considering geometry, material properties, loading conditions as inputs and corresponding deflection and stress distribution as outputs [155].

Bessa et al. developed a novel data-driven computational approach to facilitate the process of designing and modeling new material systems and structures [156]. Their approach, as represented in Figure 4, converged with different steps such as experimental design, computational analysis, and machine learning framework. The design of experiments is a fundamental step in representing the high-dimensional input variable space with a limited set of descriptors. Three types of descriptors were required for the experimental step, such as sampling material shape, microstructure material characteristics, and external factors (boundary conditions). As presented in Figure 4, the development of a database is the second step that contains all of the relevant data points required for capturing the macroscopic behavior of the material. Finally, an ML model was employed to generate a novel design structure based on the response database. Their computational approach has some challenges as their large RVE database restricts kriging because the inverse of the covariance matrix uses excessive memory with their non-optimised ML code. However, the dimensionality problem is addressed by applying a self-consistent clustering analytic strategy.

The Bayesian regression framework also offers an efficient probabilistic approach and the capability to study the unique behavior of architectured materials. It includes prior knowledge such as material composition, mechanical properties, and desired behaviors and predicts the behavior of architectured materials. For example, the data-driven computational method introduced in [158] incorporates Bayesian regression to optimize a structure that has an unpredictable response. This is an extension of the method described in [156] by incorporating additional improvements to achieve a Bayesian machine learning model that integrates a measure of uncertainty and a multiobjective optimization process. Similarly, the data-driven model in [157] adopted the approach of [158] for the design of cellular-architectured materials. Their computational data-driven methodology investigates a novel metamaterial design and tailors it to different end-use characteristics, core material choices, parameters, and fabrication techniques. As illustrated in Figure 4, the core parameters in their model are $D_1$ and $D_2$ as the diameters of the top and bottom base, $P$ as the height, and $A$ as cross-sectional area with a moment of inertia $I_x$ and $I_y$ and torsional constant $J_\tau$.

Although various ML models have been implemented to study the non-linear behavior of architectured materials with different strategies, structural analysis with inverse ML attracted most of attention as it could support reverese engineering the geometrical/material patterns. For example, Challapalli and Li [159] were used a ML model to design a 3D-printable biomimetic rod with high buckling resistance and then they expanded their model to design a novel sandwich lattice structure material with high load capacity [152]. Furthermore, Bastek et al. [160] proposed an ML-based inverse design framework to predict different truss lattice structures with data obtained from FEA simulations. After training the model, it can be used to produce different lattice structures depending on the desired level of target stiffness. They demonstrated that the combination of stochastic and physics-guided neural network models could provide a

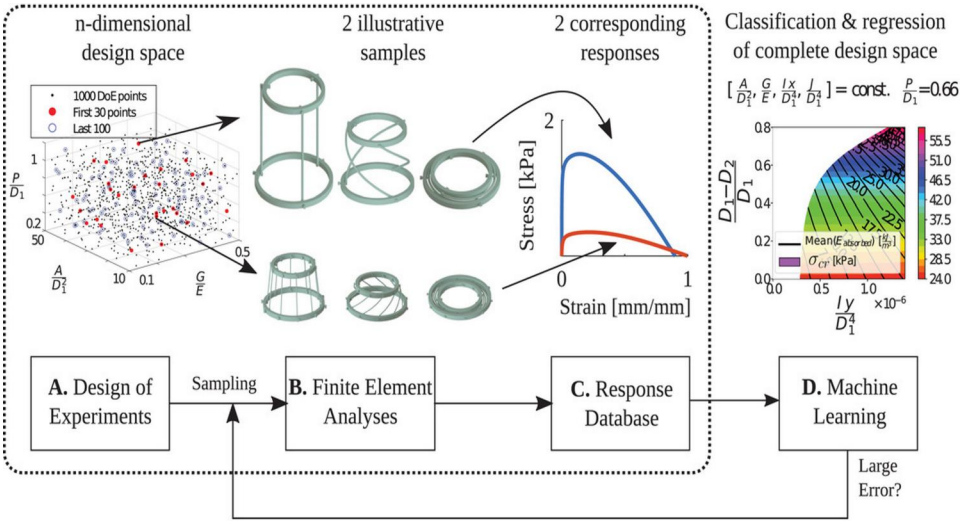


Figure 4. A data-driven computational approach for design and modeling of novel architectured materials [157].

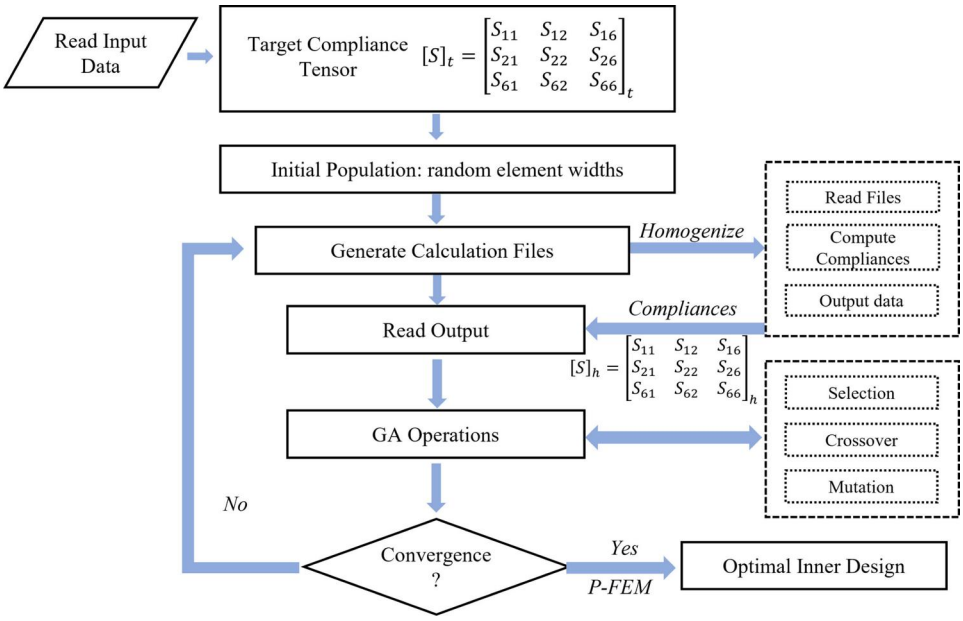


**Figure 5.** A Combined genetic algorithm and homogenization-based inverse design framework for novel architectured materials [161].

robust inverse design after the completion of training. Additionally, Dos Reis et al. [161] introduced inverse engineering for architectured material design merging genetic algorithms with discrete elements homogenization schemes that incorporated the target compliance matrix. The approach, as presented in Figure 5, identifies internal material patterns that meet all the compliance matrix standards. As presented in Figure 5, the framework consists of three different phases; (i) the initialization phase, (ii) the core computations phase, and (iii) the results and validation phases. The core computation involves the integration of asymptotic homogenization and genetic algorithm techniques. These two methods are used to locate internal material structures that effectively meet various target macroscale material characteristics. The final phase involves the validation of the results to determine whether the model has reached convergence. If convergence is achieved, the ideal internal design is produced; otherwise, the core computational phase is repeated. Although the model can save computational costs while effectively reflecting elastic behavior, it has a few limitations, including the inability to address material nonlinearities and large strain responses using the existing approach.

Hence, the research and development of architectured materials significantly benefit from the application of inverse ML methods [162–165]. These methods offer an efficient and cost-effective framework for extracting properties and optimizing structures of architectural materials to achieve the unique behaviors of these novel materials accurately.

## 5. Observations, conclusions, and future directions

The main objective of this study was to provide a review of current ML-based models that are used in the characterization, design, and analysis of materials with specific non-linear mechanical properties. In each section, ML-based material models or approaches were discussed, highlighting the advantages of techniques and research gaps to provide a comprehensive comparison between various ML algorithms. Moreover, the successful application of ML models to develop the relationship between nonlinear material properties depends on a variety of aspects, such as the selection and types of data, the nature of the specific task, and the desired characteristics to be acquired. Several ML models, including ANN models such as FFNN, CNN, and RNN, and their subtypes have prospects depending on their applications. To enhance the numerical robustness of the ML models, different extensions have been added to the general NN model, such as the convexity and Cholesky factor of the tangent stiffness matrix, to obtain the desired results.

Among all ML models, ANN-based approaches have proven to be highly effective in terms of prediction quality, flexibility, and performance to be implemented, specifically for nonlinear elastic materials. ANN models for nonlinear rete-independent materials can discover hidden and complex relationships and patterns and make predictions outside the range within large data samples. However, despite the significant potential of ANN methods in material modeling, there are still several challenges related to them. These challenges could be with the ANN models themselves or with the type of material data that needs to be analyzed. In general, tackling these challenges requires developing precise standards of material characterization that incorporate essential physical characteristics, including material symmetry [45], stability [73], and thermodynamic consistency. For example, Klein et al. [166] presented a convex input neural network model that meets the polyconvexity requirement, implying the ellipticity of the constitutive model and hence maintaining the material stability. This approach is a subset of FFNN used in [24] by adding a material stability concept. They also expanded their previous work to construct an ML-based constitutive model for electromechanically associated material behavior at finite deformation using distinct sets of invariants as inputs [73]. This methodology

focusses on material stability, material objectivity, material symmetry, and thermodynamics consistency. Regarding numerical stability, the constitutive model developed in [40] which employs symmetric positive definite neural networks (SPD-NN), weakly implies convexity of the strain energy function and fulfills Hill's second-order work condition. Therefore, it predicts the time consistency for path-dependent and rate-dependent materials and improves numerical stability. Furthermore, it is observed several times that the incorporation of thermodynamics and other concepts based on physics into the ANN models allows us to improve the training process and better and faster convergence and accuracy.

In the concept of non-linear rate-dependent materials such as viscoelastic and viscoplastic materials, the researchers have investigated and compared the performance of various ML models for developing a robust constitutive model. In general, ANN, SVM, PINN, and RNN have been found to be the most accurate and diverse ML models for such tasks. The ability of RNN models to learn the time- and history-dependent relationships is the key concept in modeling viscoelastic, and viscoplastic materials over various loading conditions. It is worth mentioning that although other ML models such as SVM, RF, and GPR can also be effectively designed for rate-dependent materials depending on particular problems and applications, they still exhibit limitations in various aspects, which are summarized in previous sections. Many of these limitations are effectively addressed through the use of PINN which has become increasingly popular for analyzing the complex behavior of nonlinear rate-dependent materials by integrating the principles of physics and theoretical laws with the power of ML models. PINN-based models not only provide stable and high-precision models but also provide dynamic stability, material stability, objectivity, internal variable stability, and consistency.

Furthermore, the structure of Architectured materials is designed in such a way that they exhibit mechanical properties that cannot be found in naturally occurring materials. As a result, various numerical approaches including ML models have been used to understand, develop, and optimize the complicated non-linear correlations between mechanical characteristics and various geometric design parameters and the parent materials of these materials. The recently designed ML models for nonlinear architectured materials include ANN, FFNN, CNN, DNN, GANs, and the inverse design framework. Inverse ML models are among the models that have the potential to develop appropriate internal structures to study the desirable mechanical behavior of architectured materials by reverse engineering. To develop innovative and novel architectures for materials with tailored characteristics, these models consider enormous amounts of data, identify patterns, accelerate design processes, and make the designs efficient and cost-effective. It is also worth mentioning that there are still certain obstacles in this area that requires further research in future including data availability, limited and noisy data, generalization, model selection, and model validation.

It is also noted that the ML models in conjunction with optimization algorithm techniques provide multiobjective functionalities that add aspects to the learning process, resulting in improved convergence, robustness, and accuracy. Some data-driven models will also make it possible to have a very optimal framework and model, and enhance the generalization ability by implementing topology optimization as well as other high computational numerical approaches. For example, the residual U-net (ResUnet) is used to generate more accuracy during training for small datasets and it produces more robust performance and enhances segmentation accuracy when low-level and high-level information are combined for training [167]. Furthermore, the model performance could be further enhanced by incorporating CNN visualization techniques to identify several mechanical characteristics such as modulus, strength, and toughness, as well as experimental parameters (crack direction and orientation, composite design limitations) using FEM simulation.

A PINN is another key future direction for the field when employing ML-based models integrate engineering design and basic physical rules as a source of training data. It uses partial differential equations for the loss function to efficiently integrate ML with mechanical design. The focus of this integration is to enhance efficiency by improving the generalizability of the model in mechanical materials and allowing the solution of a wider spectrum of problems with higher target accuracy. Hence, many ML-based models have been reviewed for their characterization and application in the design of mechanical metamaterials. Each model has specific applications and can have a different perspective by optimizing various parameters and merging different algorithms.

Finally, the authors are aware of the plenty of current/ongoing research in this area that makes the conclusion of this topic complicated. However, we believe this comprehensive summary of the key ML-based models with highlights of their suitability for different types of material properties could be specially a useful initial point for early career researchers to start their research in this fast growing field.

## Disclosure statement

No potential conflict of interest was reported by the author(s).

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