Machine Intelligence in Metamaterials Design

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Abstract

Machine intelligence continues to rise in popularity as an aid to the design and discovery of novel metamaterials. The properties of metamaterials are essentially controllable via their architectures and until recently, the design process has relied on a combination of trial-and-error and physics-based methods for optimization. These processes can be time-consuming and challenging, especially if the design space for metamaterial optimization is explored thoroughly. Artificial intelligence (AI) and machine learning (ML) can be used to overcome challenges like these as pre-processed massive metamaterial datasets can be used to very accurately train appropriate models. The models can be broad, describing properties, structure, and function at numerous levels of hierarchy, using relevant inputted knowledge. Here, we present a comprehensive review of the literature where state-of-the-art machine intelligence is used for the design, discovery and development of metamaterials. In this review, individual approaches are categorized based on methodology and application. We further present machine intelligence trends over a wide range of metamaterial design problems including: acoustics, photonics, plasmonics, mechanics, and more. Finally, we identify and discuss recent research directions and highlight current gaps in knowledge.

Keywords Metamaterials · Artificial intelligence · Machine learning · Neural Networks · Evolutionary algorithms · Surrogate modelling · Optimization

Contents

1 Introduction

1.1 Introducing Metamaterials

The properties of metamaterials are a function of material architecture and as such, metamaterial properties are not solely related to the properties of material constituents. Properties can therefore be controlled and manipulated by changing metamaterial 'unit cell' topology and while the bulk properties of the constituent materials have influence, these properties are often not the sole dominating variable used in designing metamaterials. When designing with respect to topology, the properties of metamaterials can be customized within a very large design space, and this is one of the reasons for the exponential growth in metamaterials R&D across the breadth of modern engineering. Metamaterials can be categorized according to four main objective based areas: mechanical, acoustic, optical and electromagnetic, [1].

The mechanical properties of metamaterials are of interest as the manipulation of architectures has been found to enable a very wide range of properties and behaviors. Design by computation can improve the consistency of metamaterial functionality and fundamentally desirable characteristics, such as improved material longevity, high mechanical energy absorption, and unique modes of load-controlled deformation, can be made possible by initially computing the outcome of architectural iterations to the metamaterial structure. The process is two-fold as both structure and composition are best if conjointly optimized, typically with a specified design objective. This bilateral approach is an enabler for the development of intentionally distinct mechanical properties and behaviors with significance in many generic and niche areas of application [2]–[5]. Mechanical metamaterials are often analyzed via normalized properties as a function of their relative densities through the generic relationship shown in Equation 1, where P^* is an apparent mechanical property of the metamaterial including any extant air space (e.g. E (apparent elastic modulus), σ_y (apparent yield strength), G (apparent shear modulus), etc.), P_s is the mechanical property of the solid constituent material only (i.e. the bulk property of the material assuming no air space), ρ^* is the apparent density of the metamaterial (i.e. the density per unit volume including air space), ρ_s is the density of the constituent solid material only, and C and d are adjustable constants (mathematical correction factors). The presence of the mathematical correction factors C and d clarifies that the relationship between density and properties in mechanical metamaterials is not always linear. Here, $\left(\frac{\rho^*}{\rho_s}\right) = \overline{\rho}$, and $\overline{\rho}$ is the relative density of the metamaterial, while the relative mechanical property $\overline{P}$ is equal to $\frac{P^*}{P_s}$.

$$\frac{P^*}{P_s} = C\left(\frac{\rho^*}{\rho_s}\right)^d \tag{1}$$

Mechanical metamaterials are often characterized by the type of basis structure they exhibit, Figure 1. As seen in this figure, structures can be beam based (also strut based), plate based, or minimal surface based. Beam based structures are essentially beams or struts that connect at common nodes (ends). The mechanical efficiency of a metamaterial is understood as $\overline{P} \propto \overline{\rho}^d$. As discussed by [6], the mechanical efficiency of beam based mechanical metamaterials is related to the nodal connections between beams (Maxwell's rigidity), as $b - 2j + 3 = s - m$ and $b - 3j + 6 = s - m$, for 2D and 3D respectively, where b is the number of beams (or struts), j is the number of nodes in connection, s is the number of self-stress states and m is the number of mechanisms. According to these forms, in 2D $b \geq 4$ and in 3D $b \geq 6$ for the case of stretching domination. When stretch dominated, beams are sufficiently 'thin' (with a low $\overline{\rho}$). $\overline{P} \propto \overline{\rho}^1$, for stretch dominated and $\overline{P} \propto \overline{\rho})^{1.5\to2}$ for bend dominated. When $\overline{\rho}$ is high (i.e. the beams are sufficiently thick) this scaling law no longer applies as the geometrical features of the nodes play a more significant role in controlling $\overline{P}$. While beam based structures are always essentially of the open cell form, plate based structures can be either open cell or closed cell structures. The plate based metamaterials are built up by connected thin walled sections that connect at vertices. Unlike beam based structures, which bear load more effectively along the beam axes, thin walled structures have a multi-axial resistance to loading, and when $\overline{\rho}$ is sufficiently low, $\overline{P} \propto \overline{\rho}^1$ as they are effectively stretch dominated at low relative density. Finally, minimal surface based metamaterials are comprised of curved shells where the mean curvatures are zero ($\frac{\kappa_1+\kappa_2}{2} = 0$) and the Gaussian curvatures are less than zero ($\kappa_1 \cdot \kappa_2 < 0$). Since minimal surface structures have no connections at nodes or vertices, like beam or plate based structures, respectively, they benefit from reduced stress concentration points when loaded.

While beam based, plate based and minimal surface based classifications are based on *geometry type*, mechanical metamaterials are also commonly classified based on *geometrical behavior*. A simple set of examples include pentamode, auxetic and negative stiffness, which are each characterized by the Poisson's ratio [7], ν, a ratio of transverse strain (ε_t) to axial strain (ε_a) such that $\nu = \frac{\varepsilon_t}{\varepsilon_a}$. A pentamode material exhibits the behavior of an ideal fluid and phenomenologically, a solid pentamode structure retains a constant volume under loading, which means that the Poisson's ratio remains at a constant value, similar to that of an incompressible fluid ($\nu = 0.5$). Recognizing this it can be noted from Lamé's relation [8], Equation 2, where E is elastic modulus and K is the bulk modulus, that $\frac{E}{6K}$ diminishes $\to 0$. Auxetic metamaterials are those where the Poisson's ratio is negative, i.e. $\nu < 0$. Here, an auxetic metamaterial is stretched, it becomes wider, while when compressed it becomes thinner, behaviors that are atypical to most materials. Negative stiffness metamaterials are those that deform in opposition to the direction of the applied force, resulting in material instability when unconstrained. When constrained, the same material can be stable [9] since within the allowable Poisson limits

$-1 < \nu < 0.5$, stronger ellipticity from constraint results in reduced conditions for stability, Equation 3, where G is shear modulus.

$$\nu = \frac{1}{2} - \frac{E}{6K} \tag{2}$$

$$-\infty < E < \infty \text{ or } -\frac{4G}{3} < K < \infty \tag{3}$$

A third method of classification that is commonly used for mechanical metamaterials, beyond those just discussed is based on *mechanical performance*, where performance criteria based on relationships similar to those discussed in Equation 1 form the the basis for objective oriented design. Common examples of coupled relationships include maximized strength, stiffness, and energy absorption, alongside minimized mass. An example form for coupled stiffness maximization with mass minimization is shown in Equation 4, where V is the total volume of the structure and σ is the engineering stress, m is mass, and U_e is the elastic strain energy, which is itself determined through Equation 5.

$$\frac{E}{\rho} = \left(\frac{\sigma^2 V}{2U_e}\right)\left(\frac{m}{V}\right)^{-1} \tag{4}$$

$$U_e = \int_0^{\varepsilon} \sigma d\varepsilon \tag{5}$$

Acoustic, electromagnetic and optical metamaterials are each controlled through the refractive index, $n = \frac{c}{v}$, where c is the speed of light and v is the phase velocity of light. In each case, the properties of metamaterials can be controlled by rationally designing the structure to have variability in the refractive index, which in turn results in a specific property outcome. As waves travel through a material, the refractive index n is a function of the wave frequency, ω. Acoustic metamaterials are able to direct and redirect sound waves in ways that are ordinarily unachievable in conventional materials. The two main inherent material properties that control sound wave propagation in materials are density (ρ) and bulk modulus (K). Metamaterials function on the basis of structure and as such, by altering the structure and architecture of a material, both ρ and K can be manipulated, such that an engineer can purpose-design a metamaterial to control the directing/redirecting of sound waves. Acoustic pressure is connected to ρ according to Equation 6, where v defines the acoustic particle perturbation, and t is time. Additionally, p and K are related as the motion of a non-viscous fluid is directly connected to K, which acts as a scaling constant for material compressibility. The conservation of mass is assumed in the continuity Equation 7, where the propagation of acoustic waves is taken to be isentropic. Combining therefore, Equations 6 and 7, yields the scalar wave equation Equation 8. As such, changes in the direction of waves at interfaces are controlled by the acoustic wave velocity which is described as $c = \sqrt{\frac{K}{p}}$, while the reflection and transmission amplitudes of waves at interfaces is controlled by the acoustic wave impedance, which is described as $Z = \frac{p}{v} = \sqrt{K\rho}$, [14]. As such, both K and ρ are evidently important parameters in the control of sound waves through solids, and are analogous to the electromagnetic parameters of permittivity (the electric component of light), ϵ, and magnetic permeability (the magnetic component of light as a function of wave frequency, ω), μ, such that in the electromagnetic sense, $c = \sqrt{\epsilon\mu}$ and $Z = \sqrt{\frac{\mu}{\epsilon}}$ [15]. Many such electromagnetic parameters are effectively algebraically derived from the following two relations, $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$, and, $\mu(\omega) = \mu_1(\omega) + i\mu_2(\omega)$, where 1 and 2 indicate properties relative to the different phases of the metamaterial (whether they be matter and matter, or matter and air). Electromagnetic metamaterials have many potential areas of application, including as cloaking devices, in lens technologies, for antennas, and more. One particularly interesting property of certain electromagnetic metamaterials is the ability to exhibit a negative refractive index. Conventionally, the refractive index is always positive, indicating that light, or electromagnetic waves, bends towards the normal when it enters the material. Metamaterials with a negative refractive index will not bend light, or electromagnetic waves, in this way and phenomena such as negative refraction are possible specifically by achieving $\varepsilon(\omega) < 0$ concurrent with $\mu(\omega) < 0$. Since the refractive index is $n(\omega) = \sqrt{\varepsilon(\omega)\mu(\omega)}$, this would result in an index $n(\omega) < 0$, [16].

$$\rho\frac{\partial v}{\partial t} = \nabla p \tag{6}$$

$$\frac{\partial p}{\partial t} + K\nabla \cdot v = 0 \tag{7}$$

$$\frac{\partial^2 p}{\partial t^2} = \frac{K}{\rho}\nabla^2 p \tag{8}$$

Many acoustic metamaterials contain air, and this should be factored into our overall understanding of sound transmission. While the effective density ρ_{eff} of a two component composite can be linearly volume averaged, Equation 9, where ρ_1 and ρ_2 are the material densities of components 1 and 2 and V_1 is the volume fraction of material 1, there is the underlying implication that both composite components can move together under wave motion. This is nevertheless generally not the case, as once the wave frequency surpasses the natural frequency of one of the two components, motion becomes out of phase and thence, relative [17]. A mathematical consideration to this issue has been discussed by Pierre and co-workers [18] who modeled the concept using a cylindrical pipe and spring connected materials separated by air, a toy model that could also be used to evidence negative effective density, Equation 10, where r is the radius of the material parts in the cylinder, e is the thickness of the same parts, M_{eff} is the effective mass, ρ_0 is density, S is total section area

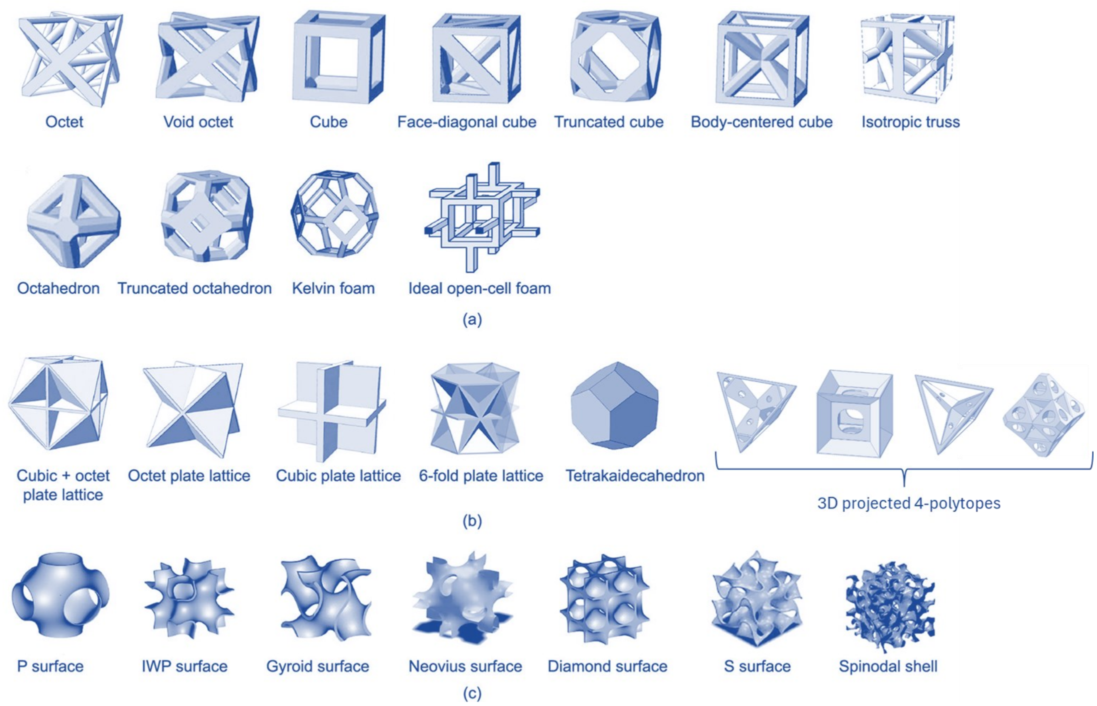

Figure 1: Examples of mechanical metamaterials based on geometry type. Illustration of 3D (a) beam-based, (b) plate-based, and (c) minimal surface-based topologies. Reproduced from [6], [10] with permission under the CC-BY licence.

($S = S_1 + S_2$), and d is the distance between material layers.

$$\rho_{eff} = V_1\rho_1 + (1 - V_1)\rho_2 \tag{9}$$

$$\rho_{eff} = \left(1 - \frac{e}{d}\right) + \frac{M_{eff}}{Sd} \tag{10}$$

Metamaterials are an emerging class of cellular materials that has attracted interest since their unique properties can be rationally designed. The design process is exacerbated and enhanced through the use of computer-aided tools for optimization, coupled with experimental measurements for validation [19]-[20]. The complexity of metamaterials creates opportunities for vastly extended design spaces, which in turn encourages more refined time-saving methods such as machine intelligence [21]-[22].

1.2 Machine intelligence and metamaterials: a growth in interest and practice

Over recent decades we note a peak in interest in the use of Artificial Intelligence (AI) and Machine Learning (ML) techniques for metamaterials engineering and design, following their successful implementation in other branches of engineering [23]–[25]. Examples include neural networks and evolutionary algorithms, which offer speedier solutions to problems with lower computational costs. High-complexity problems with a large number of design variables, such as is evident in the design of metamaterial architectures, take advantage of the fast and robust nature of AI algorithms. Metamaterial design has been shown to be accelerated through the use of ML algorithms [26] when compared against more traditional methods such as trial-and-error, and analytical physics-based approaches. New technologies that have been introduced to the field allow not only quicker solutions, but also the identification of unseen trends between the design variables and metamaterial performance [27]. There is an ever-growing desire for novel metamaterials with unique behaviors and this encourages designers to come up with new methods to further speed up the development and discovery of metamaterial architectures. As reported in [28], this requires a framework that automates the design process while concurrently increasing the rate at which the new structures are evaluated. Such frameworks can be created using a variety of AI techniques. In fact, it is now evident that AI can contribute significantly towards the future success of new metamaterials by automating labor-intensive discovery processes, and finding patterns that were previously unrecognized [29]–[31]. There are several diverse ML articles and reviews that have been published in recent times in the area of materials science and engineering, for example on glasses [32], energy materials [33], polymers [34], composites [35], additive manufacturing [36]-[37], continuum materials mechanics [38], and bio-inspired materials [39].

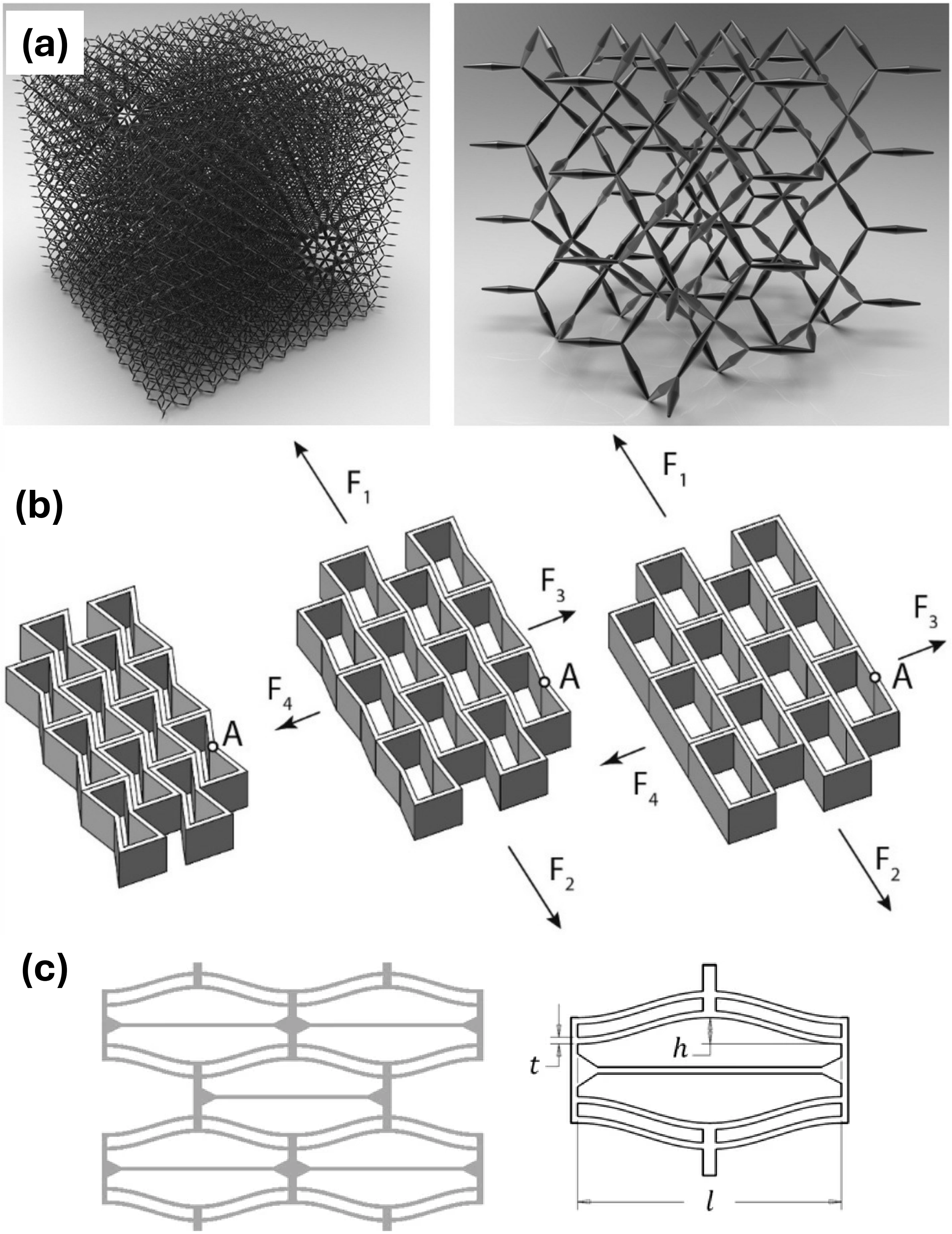

Figure 2: Examples of mechanical metamaterials defined by geometrical behavior (a) pentamode [11], (b) auxetic [12], and (c) negative stiffness [13]. Reproduced with permission under the CC-BY licence.

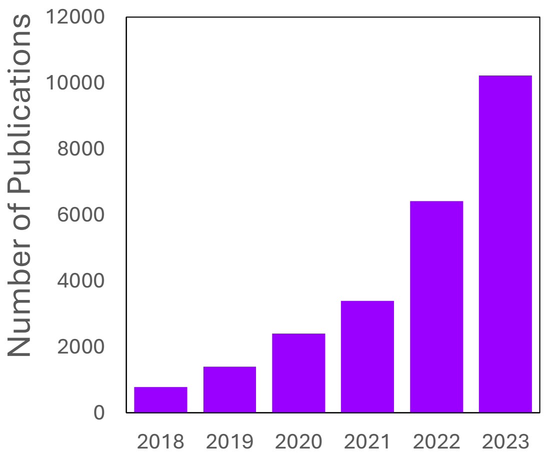

Figure 3: Distribution of publications by year which shows the increasing research trend of using ML, AI and nature-inspired optimization solutions for metamaterial applications.

1.3 Highlights from recent reviews on the AI/ML based design of metamaterials

While there are numerous reviews focusing on various classes of metamaterials and their design processes, there are only a few that consider the use of AI and ML technologies. Emergent trends in the literature inform us that the majority of current work focuses on surrogate and inverse design models, with the aim of replacing numerical analysis techniques. Nevertheless, there is seemingly still no consensus as regards the techniques suited for specific design tasks and generally, the literature lacks guidance on the *de novo* design of lattice metamaterials [40]. The increase of community interest in AI and its application to metamaterials science and engineering is evidenced by an exponential increase in research publications since 2018. Figure 3 illustrates this rise and considers published scientific work where AI and ML have been used in conjunction with metamaterials engineering.

The first review detailing metamaterials design by AI was by Choudhury *et al.* [41] in 2015. Here, they considered the metamaterial-based design of broadband antennas. Their comprehensive review discusses the applications of evolutionary algorithms that in broadband antenna design, are primarily used for solving optimization problems. Most other review papers are more recent, with the majority published from 2020 and beyond. Wang *et al.* [42] reviewed the use AI in the context of additive manufacturing. They summarize recent trends in the design of topologically optimized metamaterials and structures that are made by additive manufacturing. More specifically, they discuss the use of AI and ML techniques as methods for the development of high performance materials and customized mechanical parts. Jia *et al.* [43] summarized AI applications as a means to designing smart metamaterials. In their review, they emphasize the challenges that AI-enabled structures would face in terms of design, analysis and fabrication. Their review furthermore discussed the future trends and limitations of ML-based data-driven approaches. Bonfanti *et al.* [44] reviewed data-driven development in the context of metamaterials manufacturing techniques. They also considered other architected structures as well as biomimetic materials. Their review focused fundamentally on the mechanical applications of such structures. A few other reviews available in the literature concentrate on analyzing the AI techniques themselves and on how they are specifically exploited to generate optical metamaterials. So *et al.* [45] review on deep learning approaches for designing nanophotonics provided a detailed analysis of deep neural networks that were suitable for solving inverse design problems. Another 2020 review by Zhang *et al.* [46] summarizes machine learning and evolutionary algorithm based design and optimization techniques for the intelligent development of photonic devices. A more recent review by Picinotti *et al.* [47] discussed the use of AI in photonics while also considering nanophotonics and plasmonics in significant detail.

1.4 Virtue of this current review

Although the aforementioned reviews are highly relevant and important, each review tends to have a narrow scope or application focus. In contrast, this review uses a systematic approach to provide a broad understanding of how AI and ML have been considered across the full spectrum of metamaterials (mechanical, acoustic, electromagnetic and optical). After consideration of the currently available reviews on AI/ML and metamaterials, it is our opinion that the current body of literature is missing an overall, broad comparison of AI and ML in metamaterials science and engineering. Yet, the obvious rapid development of new AI technologies indicates that a review such as this is needed, as it will summarize advancements in the field, whilst concurrently providing useful insights based on previously published knowledge. We believe therefore, that this systematic review is both timely and essential as it will help the metamaterials community identify gaps in knowledge while highlighting both current and future trends.

2 Machine intelligence: a brief overview of concepts

There is no doubt that Artificial Intelligence, Machine Learning and Artificial Neural Networks (ANN) have become buzzwords in a number of areas ranging from science and engineering to marketing. These terms are now commonly being used interchangeably to generically describe data-driven approaches and by doing so increase interest and encourage further discussion related to data analysis. While there are many definitions of AI, it may be best defined as a branch of computer science that aims to automate the smart or learned behavior of algorithms [48]. Unfortunately, to an inexperienced user, this might make it more challenging to understand the benefits these technologies can offer. Therefore, the following section aims to provide a general background knowledge that would allow the reader to distinguish and understand the basics of AI and associated methods. To keep this review relevant to metamaterials, we focus primarily on the approaches analyzed and discussed in the reviewed literature that have been utilized in metamaterials design processes. Figure 4 categorizes different AI approaches, breaking AI into the subsets of Nature Inspired Algorithms and Machine Learning, the latter of which contains the subset of Deep Learning. The following subsections of this review briefly introduce and discuss different types of machine intelligence and their bases.

2.1 Machine Learning (ML)

ML is a subclass of AI focused on the learning and adjustment of algorithms during the data processing stage. These adjustments are based on the sets of data received and the technique is commonly associated with systems that discover trends and patterns within the data under analysis [49]. Within this subclass are artificial neural networks (ANN). ANN is a statistical machine learning technique that will process data in similitude to that of the human brain. The brain consists of interconnected neurons, or nodes, in a layered pattern and the task of ANN is to mimic the neural network pattern. ANN designs an adaptive system to continuously upgrade 'the machine' by learning from errors or miscalculations. An ANN is essentially inspired by the functionality of a neuron, which is a cell that receives electro-chemical signals from other neurons, processes the information received, and then transmits the information electro-chemically to other neurons, Figure 5. ANN is programmed to be similarly constructed such that an input layer aggregates input information from connected 'neurons', which are processed in a hidden layer that is responsible for training, and an output layer, which provides output, A, based on Equation, 11, where an ANN node takes the input value, x, multiplied by weight, W, and added to the bias, b, and this is fed through the activation function, ϕ. The abstraction of layered ANN from a neuron and its alignment to the output equation is summarized in Figure 5, from [50]. ANNs solve complex problems, such as identification, classification, or recognition with high accuracy and at high speed. The ANN analyzes input data to make accurate decisions [51].

$$A = \phi(Wx + b) \tag{11}$$

Deep Learning (DL) is also a subset of ML. DL mimics the learning process of the human brain, using artificial neural networks to achieve this goal. While machine learning algorithms require human correction, DL algorithms are self-correcting through repetition and as such there is no requirement of human involvement. While ML algorithmic training needs relatively small datasets, DL algorithms use large datasets in the training process, and include both unstructured and diverse data [52].

2.1.1 Classification of ML Techniques

ML can be subdivided into three main categories: supervised learning, unsupervised learning, and reinforced learning. Supervised learning is a task-oriented technique that is trained on labeled data (considered the ground fact) to map both inputs to outputs. Although unsupervised learning is a data-driven approach, it does not require labeled data to make ground predictions during training. In reinforcement learning, certain labels are present that distinguish it from supervised and/or unsupervised learning. A reinforcement learning approach is based on the interactions between agents and their environment and it is primarily concerned with the maximization of a cumulative reward. Algorithm performance in both supervised learning and unsupervised learning, is determined by the decreases in both the loss functions and objective functions. In addition to the three categories of learning mentioned, there is the sub-category of semi-supervised learning (or, weak supervised learning) which falls between supervised and unsupervised learning. This is a broad category that is trained on both (a) labeled data (for ground predictions) and (b) unlabelled data (to determine the larger distribution of data and its shape). Supervised learning methods are utilized regularly in metamaterials design as they are considered more mature and accurate than other ML techniques [49].

2.1.2 ML Algorithms

Classical ML algorithms are the simplest type comprising multilayer models. This section defines some of the more commonly used ML algorithms that have been used in the design of metamaterials.

Linear Regression (LIR) is an elementary method for calculating a linear relationship between input and output variables. LIR does this by relating input features with a continuous output, to predict the continuous properties of metamaterials, such as refractive index, conductivity, or other mechanical parameters like the strength and modulus of mechanical metamaterials [53]. The equation for a regression model used in metamaterial design depends on the specific goals and parameters of the design problem. However, in general, regression models for metamaterial design aim to predict specific material properties or performance metrics based on the structural characteristics or parameters of the metamaterial [54]. Equation 12 is a generic form of a regression equation that can be used for the design of metamaterials:

$$A = f(X1, X2, X3, X4, ...Xn) + \epsilon \tag{12}$$

where A represents the target output to predict, f is the regression function that relates input features to the output, and $X1$, $X2$, $X3$, $X4$,... Xn are the input features or parameters that describe the metamaterial in terms of its design. These include features and parameters such as geometric dimensions, material properties, and any other relevant parameters.

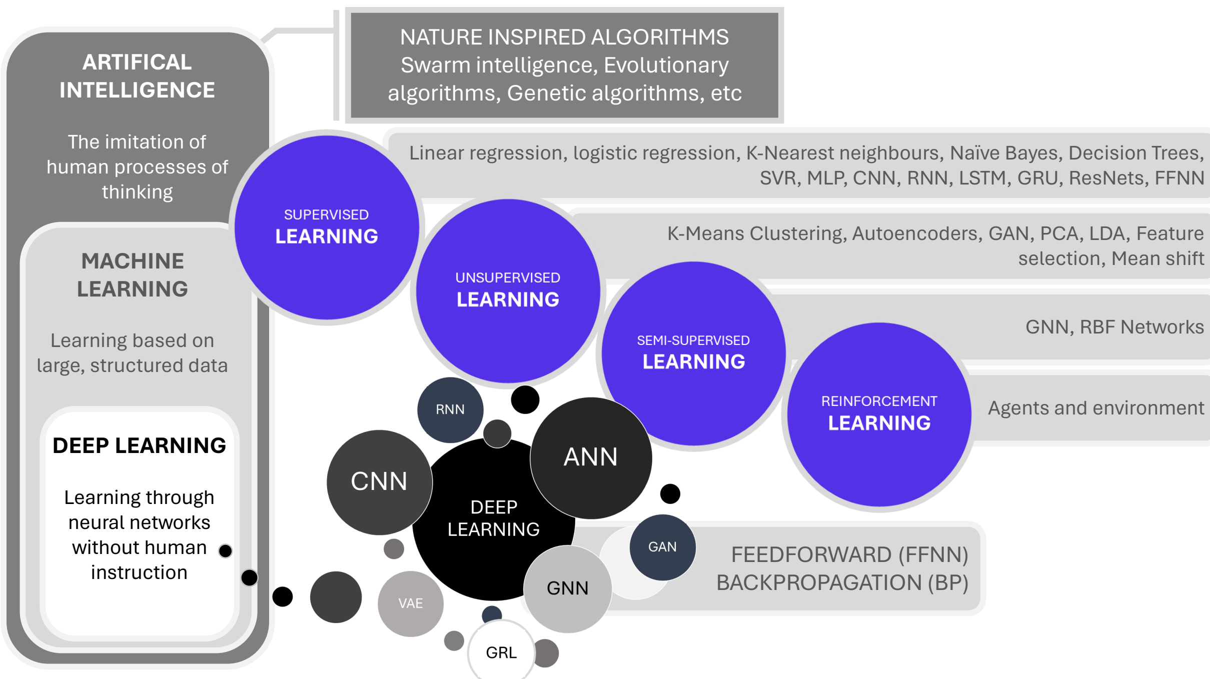

Figure 4: Categorisation of AI techniques used in the field of metamaterials. Here the following abbreviations are used: ANN - Artificial Neural Networks, CNN - Convolution Neural Networks, GNN - Graph Neural Networks, GAN - Generative Adversarial Networks, GRL - Graph Representation Learning, RNN - Recurrent Neural Networks, RBF - Radial Basis Functions, PCA - Principle Component Analysis, LDA - Linear Discriminant Analysis, SVR - Support Vector Regression, MLP - Multilayer Perceptron, LSTM - Long Short-Term Memory, GRU - Gated Recurrent Unit, FFNN - Feed Forward Neural Network

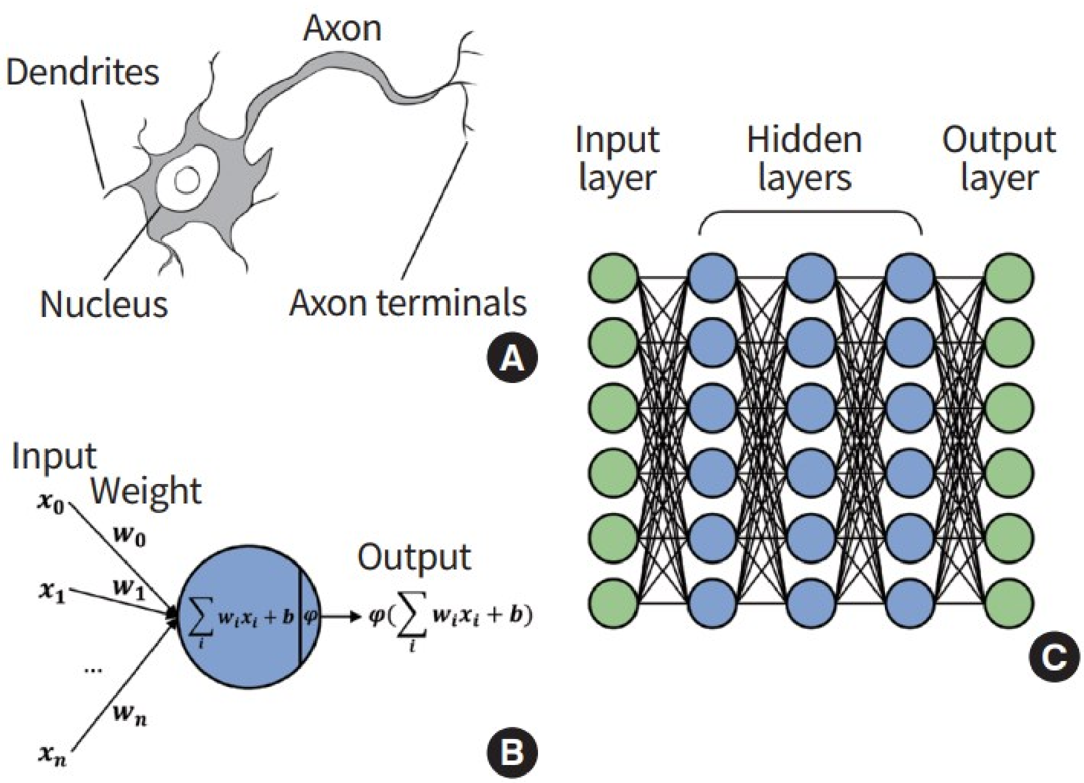

Figure 5: Overview of artificial neural network. (A) In a biological neuron, the nucleus transforms the chemical inputs from the dendrites into electric signals. The signals are transmitted to the next neurons through the axon terminals. (B) In a node (perceptron), the input values are transformed by the weights, biases, and activation functions. The output values are transmitted to the next perceptron. (C) Multilayer perceptron consists of multiple perceptrons. Reproduced with permission from [50] under the Creative Commons CC-BY licence.

$$\min_{\beta_0,\beta_1,\ldots,\beta_n} \left\{ \frac{1}{2N} \sum_{i=1}^{N} (A_i - \beta_0 - \sum_{j=1}^{n} \beta_j X_{ij})^2 + \lambda \sum_{j=1}^{n} |\beta_j| \right\} \tag{13}$$

Least Absolute Shrinkage and Selection Operator (LASSO) is a modification of the LIR algorithm. Here, an absolute penalization value is added to the loss function [55]. LASSO is used to select the most important features (parameters) when designing a metamaterial. LASSO is expressed by Equation 13, where N is the number of data points or observations in the dataset, A_i is the target variable (e.g. a material property or performance metric) for the i^{th} observation to predict or optimize., X_{ij} is the j^{th} input feature (parameter) for the i^{th} observation that describes the metamaterial, β_0 is the intercept term, β_1, β_2,..., β_n are the regression coefficients associated with the input features, and λ is the regularization parameter. This parameter controls the extent of regularization applied to the coefficients. Higher values of λ lead to greater shrinkage and hence feature selection.

Polynomial Regression (PR) is another modification of LIR. The PR method uses terms within a polynomial to find linear solutions to predict polynomial relationships between input and output variables [56]. Regression algorithms supporting nonlinear models, such as Random Forest, include the construction of multiple decision trees for the purpose of both prediction and classification. Random forests are versatile, and able to handle complex relationships between both input features and metamaterial properties by providing feature importance rankings [57].

Support Vector Regression (SVR) divides high-dimensional data space with one or more sets of hyperplanes. SVR is useful when dealing with nonlinear relationships between input parameters and metamaterial properties. A Support Vector Machine (SVM) uses the SVR algorithm for both classification and regression problems [58]. Classification tasks include identifying specific properties of a material and deciding the category within which they belong based on Equation 14,

$$Y = \text{sign}\left(\sum_{i=1}^{n} \alpha_i A_i \langle X_i, X \rangle + b \right) \tag{14}$$

where A is the predicted class label for a new input X (e.g., "+1" for positive class and "-1" for negative class), α_i are the Lagrange multipliers obtained during the SVM training process, A_i are the corresponding labels for the training data, X_i are the support vectors, which are a subset of the training data that influence the decision boundary, and b is the bias term. The key concept behind SVM classification is to determine the sign of the expression inside the 'sign' function to classify a new input into one of the two classes. This expression represents a hyperplane decision boundary that separates the classes, and the support vectors are the data points closest to this decision boundary. SVM is especially useful in dealing with non-linear separation boundaries. Such nonlinear models are very accurate, and can handle outliers better than linear regression models. Apart from regression tasks, classification is another important category in ML algorithms as it enables the classifying of metamaterials into predefined groups.

Logistic Regression (LOR) is a classification algorithm that includes a logistic loss function. In the context of materials design, it can be used to predict categorical outcomes, e.g. will a particular material exhibit a specific property or behavior [57]. Based on Equation 15, logistic regression for materials design as is,

$$P(A=1) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_n X_n)}} \tag{15}$$

where $P(A = 1)$ represents the probability that the categorical outcome A is equal to 1, e is the base of the natural logarithm (ca. 2.71828), β_0, β_1, β_2... β_n are the regression coefficients associated with the input features that allow the prediction of the probability of a positive outcome based on the material characteristics, $X1$, $X2$, $X3$... X_n are the input features, or parameters, that describe the characteristics of a material.

Numerous ML algorithms deal with both classification and regression solutions such as **Gradient Boosting** [59], **Decision Tree (DT)** [60], and **K-Nearest Neighbors (KNN)** [61]. These algorithms can be used for data representation, feature engineering, and hyperparameter selection in metamaterial design problems. In classical ML algorithms, Artificial Neural Networks (ANN) are the most vital basic building blocks based on perceptrons as a means of developing network structures by generating a stack of multiple layers of artificial neurons to establish nonlinear relationships between input and output variables, and the distribution of data [62]. As the number and depth of network layers increase, DL models showcase their capacity to provide tremendous results in numerous interdisciplinary areas including in computer science.

Multilayer Perceptron (MLP) or Feedforward Neural Networks (FFNN) are simple and perfect DL models. Information in FFNN models travels in one-way, as the name implies. Every layer in FFNN contains multiple neurons that generate output to succeeding layers, depending on the input from the preceding layers. The trainable parameters/weights are used to calculate respective neuron values and enhanced to decrease the value of the loss function [62].

Back Propagation (BP) is another general ANN method, implemented with the Gradient Descent (GD) method, and aimed at gaining the lowest value of a loss function during the training process [63]. BP functions are similar to the calculation of derivatives, while GD methods decide how to transfer the value of the loss function to a lower value. The process repeats until the value of the loss function reaches a minimum. The mathematical form of backpropagation for a feedforward neural network for metamaterial design is provided in Equations 16-25. For a given input sample, a forward pass computes the network's output $A^{(L)}$, where L is the number of layers. It calculates the activations and weighted sums in the activation function $A^{(l)}$ for each layer l from 1 to L as in Equation 16, where $f^{(l)}$ is the activation function for the layer l, Equation 17. For a Loss computation, loss is calculated between the network's output $A^{(L)}$, and the true target values Y using a suitable loss function, typically a mean squared error (MSE) for regression tasks, or, cross-entropy for classification tasks as shown in Equation 18.

Forward Pass:

$$Z^{(l)} = A^{(l-1)} \cdot W^{(l)} + b^{(l)} \tag{16}$$

$$A^{(l)} = f^{(l)}(Z^{(l)}) \tag{17}$$

$$L = \text{Loss}(A^{(L)}, Y) \tag{18}$$

Backward Pass:

In a Backward pass, gradients of the loss with respect to the weights and biases are computed to minimize the loss, Equation 19, with respect to the output of the last layer. Gradients are then computed for each layer l from $L-1$ to 1. Equation 20, and Equation 21 show the Gradient of Weighted Sum and Gradient of Weights respectively. The Gradient of Biases with respect to axis = 0 shown in Equation 22 and Equation 23 shows the activation for the previous layer.

$$dA^{(L)} = \nabla L \tag{19}$$

$$dZ^{(l)} = dA^{(l)} \cdot f^{(l)\prime}(Z^{(l)}) \tag{20}$$

$$dW^{(l)} = A^{(l-1)T} \cdot dZ^{(l)} \tag{21}$$

$$db^{(l)} = \sum(dZ^{(l)}, \text{axis} = 0) \tag{22}$$

$$dA^{(l-1)} = dZ^{(l)} \cdot W^{(l)T} \tag{23}$$

Update Weights and Biases:

Using the gradients computed in the backward pass, weights based on Equation 24 are updated as are biases as shown in Equation 25 within each layer using a gradient descent optimization algorithm, such as stochastic gradient descent (SGD):

$$W^{(l)} = W^{(l)} - \alpha \cdot dW^{(l)} \tag{24}$$

$$b^{(l)} = b^{(l)} - \alpha \cdot db^{(l)} \tag{25}$$

where α is the learning rate, a hyperparameter that controls the step size during weight and bias updates. This process is iterated until the neural network's weights and biases converge to values that minimize the loss function, effectively training the network to make accurate predictions for material design. The specific architecture and hyperparameters of the network will depend on the problem and dataset in the context of materials design.

Convolutional Neural Networks (CNN): With the exception of general FFNN and BP algorithms, CNN are the most well known DL architectures, gaining extensive attention due to their numerous applications in Natural Language Processing (NLP), and computer vision. Over recent decades, CNN have become one of the most powerful tools as they have an immense capacity for handling significant image data.

CNN are image-based DL models where an artificial neuron receives input images, assigns learnable weights and biases to various objects or aspects within the images, processes them, and subsequently processes the result as output. The input layer takes input image pixels in a matrix form and sends them to multiple hidden layers, where feature extraction is performed by a mathematical linear operation called 'Convolution'. CNN differ from simple neural networks in that the data is convolutional, which is beneficial when processing images. A CNN can be mathematically represented as a series of mathematical operations, including convolution, pooling, and fully connected layers. Equation 26 shows the convolution operation of a simple CNN architecture, where the convolution operation is $*$ and involves applying a filter (also called a kernel), W, to a 2D or 3D input image X, resulting in an output feature map Y. i and j represent the spatial coordinates of the output feature map, m and n represent the spatial coordinates of the filter, and $\cdot$ defines element-wise multiplication [64]. The architecture and the number of layers in a CNN can vary significantly depending on the problem at hand, and more complex architectures often involve additional components like skip connections, batch normalization, and dropout to improve training and generalization performance.

$$Y(i,j) = (X * W)(i,j) = \sum_m \sum_n X(i+m, j+n) \cdot W(m,n) \tag{26}$$

CNN require far less pre-processing as compared to other ML classification techniques. While traditional techniques use hand-engineered filters, with abundant training, CNNs can learn these filters/characteristics [65]. In materials design problems, CNN are good for describing material properties through their ability to extract features at various hierarchical levels [64]. It is not solely materials that have various features at innate hierarchical levels, but this concept is universal e.g. sound, language, matter, etc [66].

Recurrent Neural Networks (RNN) have also gained popularity along with CNN through their capacity to deal with sequential information. There is the main difference between CNN and RNN is that in CNN, input and output are considered to be independent of each other, while RNN analyze the sequential data, and the output depends on the latter and previous sequence, using memory to decide the output of each layer. CNN might not deal with sequential tasks, for example, it would be difficult for CNN to emphasize the sequence of information to predict the next word in an incomplete sentence if the sequence of sentences is absent. RNN deals precisely with these types of sequential problems. The gradient manipulated by BP can be vanished or expanded in RNN [67]. To meet this challenge, various types of mechanisms have been developed such as Gated Recurrent Units (GRU), Long Short-Term Memory (LSTM) [68], Attention [69], and ResNet [70], growing the power of RNN in different natural language processing problems for instance speech processing and language translation. RNN are also gaining more routine use in scientific tasks such as *de novo* protein design and protein folding.

Generative Adversarial Networks (GAN) are based on generative algorithms and are used to create new data points based on real data distributions. GAN are a successful architecture and includes two separate neural networks: the 'Generator' and the 'Discriminator' [71]. The task of the generator is to create new 'fake' data points, while the discriminator matches these 'fake' data points with the existing data. During the training process, both the generator and the discriminator contend as the generator produces new genuine but 'not real' data points as a part of its aim to fool the discriminator. Concurrently, the discriminator discriminates the real data from the fake data as effectively as possible. The mathematical form of GANs in the context of material design involves two main components: the generator and the discriminator as shown in Equation 27 and 28 respectively. The generator G takes random noise z as input and produces fake data M_{fake} as output:

$$M_{\text{fake}} = G(z; \theta_g) \tag{27}$$

M_{fake} represents the generated material structure or property, z is the input random noise vector, and θ_g represents the parameters of the generator neural network. The discriminator D evaluates whether an input data point M is real or fake:

$$D(M; \theta_d) \tag{28}$$

$D(M; \theta_d)$ represents the probability that M is a real material structure or property, θ_d represents the parameters of the discriminator neural network. GAN achieve convergence at the moment when the Nash equilibrium is held between the generator and the discriminator. The method of balancing the performance of both networks is similar to the equilibrium process in a physical system that includes both forces of attraction and repulsion, which shows GAN can likely also describe physical phenomena. Conditional GAN (CGAN) is a type of GAN, that generates data under controlled characteristics or conditions, using labels as a control variable [72]. The image-to-image translation is an example of CGAN that use an original image as a control variable in the generator [73].

Variational Autoencoders (VAE) include a single neural network to encode the input information into a latent code, after which the output data is reconstructed by decoding the latent code [73]. It is another type of generative model used for tasks such as feature extraction, data generation, and dimensionality reduction. While VAE have not typically been used in metamaterial design, they can play a role in assisting with certain aspects of the design process, such as in generating new material designs, exploring latent spaces, or in optimizing the material properties [74].

Principal Component Analysis (PCA) and **Linear Discriminant Analysis (LDA)** are dimensionality reduction techniques commonly used in metamaterial design. While neither are direct design tools for metamaterials, they can be a valuable pre-processing step or analysis tool in the context of metamaterials research. Metamaterial design deals with high-dimensional feature spaces representing material properties, geometries, or other characteristics. PCA and LDA can be used to reduce the dimensionality of the feature space by identifying and retaining the most informative features (principal components) while discarding less important ones [75][76]. They can potentially simplify the design space and thus make it more manageable.

Reinforcement Learning (RL) is a class of ML algorithms based on environmental variations and aimed at maximizing long-term achievements. The training process focus is in finding an equilibrium between the exploitation of existing knowledge and the exploration of new territory [77].

Unlike normal neural networks, **Graph Neural Networks (GNN)** are another type of ML technique, operating on Euclidean information and acting on non-Euclidean data graphs with nodes connected by corners in unnatural orders [78]. **Graph Convolutional Networks (GCN)** are current breakthroughs in GNN and have been demonstrating the competency of GNN to learn graph embedding through the passing of messages between nodes. GCN performed outstandingly in semi-supervised classification problems that are equally applicable to both mechanics and materials design problems, including graphical structures [79]. **Radial Basis Function (RBF)** networks are a type of artificial neural network that can be applied to various machine learning tasks, including regression and classification. While RBF networks are not as commonly used as other neural network architectures such as CNN or RNN in metamaterial design, they still show potential as a valuable tool in data representation and evaluation and optimization tasks [80].

Transfer Learning is a recent breakthrough in machine learning and is a powerful tool as it recycles previous training, which can later be used for both the basic and advanced stages of machine learning. Transfer learning is a beneficial approach when the user starts from scratch. When the resources to build a model from the ground up are unavailable, using Transfer Learning, the user can benefit from a pre-existing model. The user can apply the same principles that have been used for training on similar large quantities of data, and can then modify it for a specific use case. By adjusting model parameters and feeding it new data, the model rapidly adapts and learns to classify new objects, saving computational resources and a significant amount of time [81] [82].

2.2 Nature Inspired AI Algorithms

Nature inspired AI algorithms draw inspiration from natural processes, behaviors, or phenomena in the biological, physical, or ecological world to solve complex optimization and design problems. These algorithms are often used in metamaterials design to efficiently explore vast design spaces, and to discover novel structures with desirable properties. This section will explore some commonly used nature-inspired AI algorithms in metamaterials design.

2.2.1 Genetic Algorithms (GA)

Evolutionary algorithms are a nature-inspired optimization algorithm that mimics the process of natural selection and evolution to search for optimal or near-optimal solutions in a design space. Genetic algorithms (GA), are amongst the most well-known evolutionary algorithms used in the design of metamaterials. GA have found extensive applications in the optimization of metamaterial lattice structures, especially in combination with machine learning formulations. These approaches leverage the power of GA in exploring the vast design space of metamaterials, and by combining them with machine learning techniques, the user can enhance the optimization process to discover innovative lattice structures [83].

Machine learning models, such as surrogate models or neural networks, are used to approximate an objective function that evaluates the performance of a given lattice structure. GA can then be used to optimize the surrogate model, thereby reducing the computational cost that would normally be required if evaluating each design individually [84][3]. Mathematically representing a GA for metamaterial design requires definitions of the key components that govern the optimization process. Equation 29 illustrates design as a chromosome or genome, where X represents a chromosome, which is a vector of the design parameters, and each x_i corresponds to a design parameter, such as materials properties or geometrical characteristics.

$$X = [x_1, x_2, \ldots, x_n] \tag{29}$$

In Equation 30, P_t is an initial population of N individuals (chromosomes) obtained randomly or using heuristic methods. Equation 31 shows objective function $f(X)$ that quantifies the performance of a metamaterial design based on the design parameters X. This function evaluates how well the metamaterial meets specific design objectives or constraints.

$$P_t = [X_1, X_2, \ldots, X_N] \tag{30}$$

$$f(X) : X \to \mathbb{R} \tag{31}$$

Equation 32 is used to evaluate the fitness of each individual in the population using an objective function, where $F(X_i)$ is the fitness of individual X_i.

$$F(X_i) = f(X_i), \text{ for } i = 1, 2, \ldots, N \tag{32}$$

Selection mechanisms such as roulette wheel selection or tournament selection can be used to choose individuals from the current population to become parents for the next generation. The probability of selection for an individual, X_i, is proportional to its fitness, $F(X_i)$. After selection, it applies crossover (recombination) to pairs of parent chromosomes to create offspring chromosomes as shown in Equation 33. A common crossover operator is a single-point crossover. The specific crossover method depends on the problem and on chromosome representation.

$$X_{\text{offspring}} = \text{Crossover}(X_{\text{parent}_1}, X_{\text{parent}_2}) \tag{33}$$

Mutations introduce small random changes to offspring chromosomes to add diversity to the population. Mutations help the user explore new regions of the design space as understood in Equation 34.

$$X_{\text{mutated}} = \text{Mutation}(X_{\text{offspring}}) \tag{34}$$

A New Population is formed by selecting the best individuals from the current population (elitism) and adding the offspring and mutated individuals as shown in Equation 35.

$$P_{t+1} = [X_{\text{elite}_1}, X_{\text{elite}_2}, \ldots, X_{\text{mutated}_1}, X_{\text{mutated}_2}, \ldots] \tag{35}$$

GA specifies termination criteria, such as a maximum number of generations or a convergence threshold based on fitness values. GA continues until the termination criteria are met. The final population consists of individuals that represent optimal or near-optimal metamaterial designs. The choice of operators, chromosome representation, and objective function, will depend on the problem at hand and the characteristics of the metamaterial design task [85].

GAs are versatile and can be used in various aspects of metamaterial design, including optimizing electromagnetic properties (e.g., achieving desired frequency responses or refractive indices) [86], mechanical properties (e.g., stiffness or flexibility) [87], etc. They are particularly useful when the design space is large, complex, and nonlinear, enabling the discovery of innovative solutions that might be challenging to find through manual design or through other optimization methods.

2.2.2 Swarm Intelligence

Swarm intelligence algorithms can be beneficial in optimizing the structure and properties of metamaterials for various applications. These algorithms emulate collective, decentralized behaviors observed in natural swarms such as bird flocks, fish schools, and ant colonies, to efficiently search across a design space, and subsequently discover novel metamaterial architectures. These systems exhibit emergent intelligence and adaptability, allowing them to find solutions to complex problems with no centralized control. Swarm intelligence algorithms emulate these behaviors to solve optimization, search, and decision-making tasks [88]. Researchers and practitioners often choose the most suitable algorithm based on the characteristics of the problem, the optimization goals, and the available domain knowledge. **Ant Colony Optimization (ACO)** is one of the most popular swarm intelligence algorithms, inspired by the foraging behavior of ants. It is used to solve combinatorial optimization problems. Ants deposit pheromones on paths, and other ants use these pheromone trails to make decisions. Over time, paths with higher pheromone levels are favored [89]. **Particle Swarm Optimization (PSO)** is another popular swarm intelligence algorithm used in metamaterial design. It is inspired by the social behavior of birds when flocking or fish when schooling. It optimizes a problem by iteratively adjusting a population of particles within the solution space. Particles move towards the best-known solution (individual best) and the best-known solution among all particles (global best) [90]. **Bee Colony Optimization (BCO)** algorithms are based on the foraging behavior of honeybees. Bees explore the solution space and communicate information about promising solutions to their hive mates. It is commonly used for solving optimization problems and is particularly effective in continuous optimization [91]. **Firefly Algorithms (FA)** are based on the flashing behavior of fireflies, where fireflies attract each other with their light. In optimization problems, fireflies represent potential solutions, and their brightness corresponds to the quality of the solution. Fireflies move towards brighter neighbors, and the algorithm converges to an optimal solution [92]. The **Bat Algorithm (BA)** is inspired by the echolocation behavior of bats used for continuous optimization and employs a population of virtual bats that search for solutions in the search space. Bats emit sound waves, and the algorithm adjusts the frequency and loudness of these waves to explore and exploit the solution space. **Cuckoo Search (CS)** algorithms are inspired by the breeding behavior of cuckoo birds, this algorithm is used for global optimization problems. It involves a population of virtual cuckoos that lay eggs in host nests. The quality of a nest corresponds to the fitness of a solution and the algorithm mimics the natural selection process [93]. The **Krill Herd Algorithm (KHA)** is based on the herding behavior of krill and involves a population of virtual krill that move collectively toward improved solutions. Krill update their positions based on both personal experience and social interactions [94]. Each of the swarm intelligence algorithms mentioned has been used for the design optimization of metamaterials, which will be discussed in Section 3. The methods are versatile and applicable to various optimization and search problems across different domains.

3 Machine Intelligence in Metamaterial Design

This section prioritizes publications where machine intelligence has been applied to solve metamaterial problems. The section begins (Section 3.1) with machine learning applications focusing on: gradient-based methods, dimensionality reduction, and other ML methods, including predominantly regression. This is followed by consideration of the application of ANN to metamaterials design (Section 3.2). ANN has a very specific set of application methods including surrogate modeling and inverse design, and as such we focus our discussion on these. Finally, we highlight papers applying nature-inspired methods (Section 3.3), which are commonly used in the design of metamaterials.

3.1 Machine Learning in Metamaterials Design

3.1.1 Gradient-Based Methods

Gradient-based methods are efficient approaches for design optimization problems comprising multiple variables. Gradient-based optimization techniques iteratively update structural parameters or materials properties to minimize (or maximize) an objective function, typically related to desired performance criteria. Algorithms, such as conjugate gradient and steepest descent, perform searches to find optimal design arrangements taking into account the prescribed constraints while minimizing an objective function [95]. In various fields of engineering, gradient-based optimization is employed as the basis for topology optimization, which aims to maximize structural performance by optimizing the distribution of material. This application includes but is not limited to automotive, aircraft, and structural engineering [4], [96]. In the metamaterials context, gradient-based nonlinear topology optimization has been shown as effective for the microscale design of elastic structures [97]. Backer and co-workers [98] use the steepest descent algorithm to optimize metasurfaces. Their approach made use of analytical simulations in the context of Fourier optics, for which gradients were evaluated using an adjoint-gradient approach. In another paper [99] metasurface designs were optimized using a level-set method to define the refractive index of a meta-atom cross-section. The objective function was then described as the difference between the desired output and the optical response of a meta-atom, and gradient descent optimization was used to seek out and find the most suitable meta-geometries. Other papers in the field employ algorithms such as gradient descent to optimize problems related to elastic metamaterial-based vibration absorbers [100], electromagnetic devices [101], photonic band gap structures [102] and acoustic metamaterials [103]. Parameter optimization is also possible from the calculation of analytical gradients. This approach is commonly used in ANN training, and gradient-based algorithms employed in back-propagation [104] are also a means by which model parameters can be adjusted [105]–[111].

Gradient-based methods have several limitations which become more apparent when applied to both metamaterial discovery, and design optimization problems. Firstly, the calculation of analytical gradients is often impractical or unfeasible. Unlike in topology optimization problems where the analytical gradients can be found using adjoint methods [101], the equations governing the behavior of metamaterials and the exact solution to these equations are usually unknown. Therefore, most metamaterial design processes rely on computationally expensive FE-based approaches that approximate the numerical gradients. Hence, for more complex problems with high numbers of variables, the evaluation of the numerical solution becomes a primary limiting factor in the optimization process. Secondly, gradient-based methods tend to get caught at local minima or saddle points, resulting in the manifestation of sub-optimal solutions. They also struggle to handle non-smooth functions, where gradients cannot be evaluated at the points of discontinuity. Consequently, the performance of gradient-based optimization may vary drastically depending on the initial estimates defined as a starting point of the algorithm. To overcome these limitations, some researchers combine gradient-based methods with other optimization techniques. For example, Boddeti *et al.* [112] reports a hybrid inverse design framework using gradient descent and gradient-free (GA) algorithms to find an optimal metamaterial structure for a thermal-photovoltaic emitter coating application. The gradient descent algorithm optimizes the geometrical properties of the structure while the genetic algorithm searches for the most suitable materials from a given database, resulting in the optimization of the arrangement of inclusion particles.

3.1.2 Dimensionality Reduction

Dimensionality reduction (DR) refers to ML approaches that are designed to reduce the number of features describing a given data set. This is achieved by either the generation of new features based on the existing ones or through the selection of key features within the set that best represents the data. A few applications that benefit from such approaches include but are not limited to, data visualization, storage, and tasks involving heavy computations. The latter is the most frequently applied in the development of metamaterials as they help reduce computational expenses during the simulation, prediction or generation of new metamaterial architectures.

A method invented and first introduced by Reuter *et al.* in 2005 [113] called 'ShapeDNA' is a technique for shape characterization based on spectral shape descriptors. It approximates the geometrical shape of any 2D or 3D object by taking the eigenvalues of its Laplace-Beltrami operator [114]. The method is simple, does not rely on previous knowledge, and is highly suitable for the retrieval of non-rigid shapes [115]. This was used as a DR technique in a data-driven mechanical metamaterial design framework as presented by Wang *et al.* [116]. The researchers showed that by approximating a complex unit cell shape with a low number of descriptors, they were able to significantly reduce computational requirements. A similar dimensionality reduction approach has been reported in the two publications by Bostanabad *et al.* [117], [118] where these researchers used spectral shape descriptors based on Laplace-Beltrami operators to reduce the metamaterial input dimensions from 2500 pixels to 16 scalar descriptors.

Another approach is to employ a principal component analysis (PCA) which is a linear DR technique that constructs a best fitting lower dimensionality subspace within the initial data space. It aims to position the linear subspace so that the data approximation error can be minimized. PCA has been used as means to reduce 5 design variables of photonic devices to no more than 2, allowing them, therefore, to reduce the optimization problem size and perform an in-depth exploration of the design space [119]. Wang *et al.* [111] further demonstrated that this technique could be used to reduce dimensionality by applying it to the latent space generated by a variational autoencoder, hence enabling visualization of the results. In the same paper, PCA was applied as a tool to cluster data points within the latent shape according to their representative metamaterial shapes and structures. A more in-depth analysis of different DR techniques has been summarized by Kiarashinejad *et al.* [120] who compare a traditional PCA with KPCA (kernel principal component analysis), a nonlinear PCA technique, and an autoencoder. They suggested that although autoencoders are more computationally intensive to train and use, the DR capabilities and performance of the approach surpass PCA and KPCA. Other less commonly applied ML algorithms for DR problems in metamaterial design include t-distributed stochastic neighbor embedding (t-SNE) [121] and the Isomap [122] algorithm and its extensions.

3.1.3 Other ML Algorithms

This section summarizes some of the less commonly applied machine learning algorithms in metamaterials design, primarily regression algorithms, which are used to determine regression trends within the available data. Kurniwati *et al.* [123] employed random forest regression algorithms to build models that were able to predict antenna parameters, such as gain, Voltage Standing Wave Ratio (VSWR), bandwidth, and return loss, based on the metamaterial structures and their distinct performance parameters as applied to training in the algorithm. Their work suggests that a predictive approach such as was used, enabled a reduction in computational time, when compared against conventional optimization techniques. Liu *et al.* [124] presented a similar justification for the use of machine learning algorithms. The research team reported that simple regression algorithms were more accurate and efficient for predicting the performance of graphene-based metamaterials, as compared to ANN. Their work compared Decision Tree, Extra Tree, KNN, Random Forest algorithms and ANN performance for the forward and inverse design of photonic devices [125]. Mukherjee *et al.* [126] considered ANN, complex tree, weighted KNN. These are referred to as soft computing techniques and the group used these to classify metamaterial-based defected photonic crystal structures. Clustering methods were used by Moon *et al.* [121], specifically K-Means clustering, to design metaplasmonic biosensors with negative index metamaterials. Further, nonlinear programming has been shown by Bacigalupo *et al.* [127] to be an effective method for designing acoustic metamaterials. Other forms of less common forms of metamaterial optimization besides Clustering techniques include Nelder-Mead and Bayesian, [128], which has been used to optimize structure and also to optimize wave band gaps in mechanical metamaterials, [129]. Bayesian machine learning has been reported as a method for the design of super-compressible micro scale mechanical meta-structures, [130], while Gaussian Radial Basis Function (RBF) networks used together with Quasi-Monte Carlo sequences [131] are a form of multiple optimizations, which is also noted in [132] where CNN (Resnet50) and Monte Carlo methods were used in parallel for the optimization of actuators.

3.2 Artificial Neural Networks in Metamaterials Design

In this section, papers that focus on the use of artificial neural networks (ANN) in metamaterials design are discussed. The section is broadly divided into: surrogate modeling (Section 3.2.1), inverse design (Section 3.2.2), and a presentation of less commonly used methods (Section 3.2.3).

3.2.1 Surrogate Models

Artificial neural networks (ANN) are commonly used for building surrogate models. ANN are highly suitable for this application as they have the ability to learn and predict outputs based on the training data supplied. According to [133] artificial neural networks can approximate any continuous function, making them suitable for use alongside numerical methods such as finite element analysis (FEA). Further, designers can benefit from the abundance of available network architectures that can further be customized to meet predictive modeling needs. As FEA is commonly used for structure-function optimization in metamaterial design, multiple publications can be found discussing their research in terms of replacing this numerical method with ANN-based solutions.

Some researchers use ANN as a tool for the analysis and prediction of mechanical properties. Gu *et al.* [134], for example, have shown that this unconventional approach to optimization enables the design of metamaterials without the need for complete micro-structural data, also referred to as coarse-grained modeling. Using a CNN architecture to speed up the process of predicting mechanical response, they report that while FEA methods required a 5 day compute time, a trained ANN-enabled framework required only 1 minute to compute 100,000 microstructures. Importantly, Gu and co-workers also showed that the final characteristics for material placement in an optimized tough-structure, are those that localize in the areas of crack opening, as shown in Figure 6. This corresponds well to the placement of energy absorbing material at the site of splits and openings in natural structures such as in insect wings, [135].

In an aligned paper by Xue *et al.* [136], similar findings are reported. Here, they showed that a surrogate ANN model reduces computational time by two orders of magnitude when compared to finite element simulations. Their work employed a single hidden layer architecture to predict the nonlinear mechanical behavior of hyperelastic metamaterials. Constitutive models can be used to analyze hyperelastic lattice structures [137]. Here, the authors developed models based on a feedforward ANN architecture, and inform that in some cases, higher accuracy results were achieved as compared to the analytical model. The work of [137] provides clarity on the distinctness of the

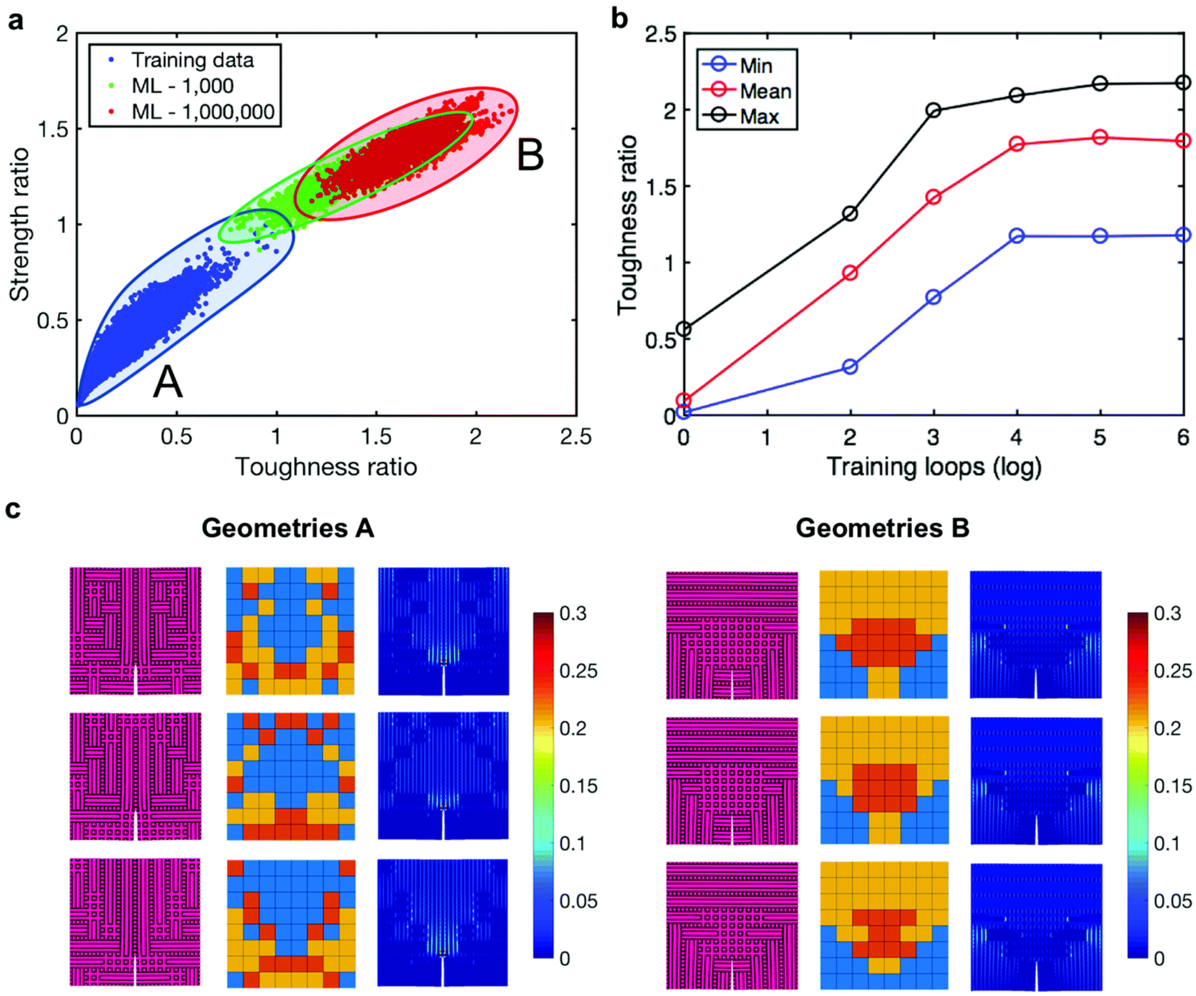

Figure 6: Machine learning generated designs. (a) Strength and toughness ratios of designs computed from training data and ML output designs. The strength ratio is the strength normalized by the highest training data strength value. The toughness ratio is the toughness normalized by the highest training data toughness value. The ML output designs are shown from training loops of 1000 and 1000000. Envelopes show that ML material properties exceed those of training data. (b) Effects of learning time on ML models for minimum, mean, and maximum toughness ratio start to converge as training loops increase. (c) Microstructures from partitions A (lowest toughness designs in training data) and B (highest toughness designs from ML) in part (a) of the figure with corresponding colors for unit cell blocks (blue = U1, orange = U2, yellow = U3). Also shown in the right-most columns for designs A and B are the strain distributions, which show lower strain concentration at the crack tip for the ML-generated designs. Reprinted with the permission of [134] under a Creative Commons CC-BY licence.

deformational, $\boldsymbol{F}$, and 1st Piola-Kirchhoff stress $\boldsymbol{P}$ states of a baseline structure described as an X-cell, for uniaxial, biaxial, planar, volumetric and shear cases, Figure 7. The work highlights the importance of algorithm training with respect to deformational behavior, as the authors note that equal stress and deformation for each strut of an X-cell is only true for a volumetric loading case, and as such, structure organization has to be considered in the context of its utility. Here, the plots correspond to 3×3 matrices denoted by the colors in the legends.

Similar surrogate models have been used for the analysis and simulation of high frequency electronic products such as antennas and antenna arrays. In a paper by [138], Saha *et al.* discuss a data driven approach in analyzing split ring resonator metamaterials and reveal that high accuracy can be achieved using a surrogate model. Another team [139], [140] demonstrated ANN predictions of permeability and permittivity in split ring resonator type (SRR) metamaterial designs. ANN-based models are also shown to appropriately replace commercially available FE packages and other analytical models as a design tool for electromagnetic metamaterials [141], meta-optics components, and optical devices [142]–[145]. Wu *et al.* [5] in addition considered the design of 1D acoustic metamaterials using an artificial neural network-based surrogate model. In their work, they found the method was useful even for aperiodic metamaterials, and noted that their approach neither requires a predefined number of unit cells to function effectively nor is there a need for the user to understand the physical model well for it to work.

Convolutional networks are an attractive basis for surrogate modeling as they have the ability to recognize patterns within a design space, irrespective of pattern location. Geometrical features such as chamfers or fillets can be easily distinguished and optimized to reduce stress concentrations. In a paper by Garland *et al.* [40], machine learning methods were developed to be Pareto Optimal, an approach that took on two objectives: wave propagation through a material, and the elastic modulus. They found the best possible trade-off between the two without stipulating any particular claim about which combination is best. Essentially, a Pareto Optimal approach does not allow the improvement of one objective, without leading to the worsening of the other objective. In Figure 8 (a) their initial results from 1000 random designs can be seen and in (b) both numerical and experimental validations of three of their final generated designs are shown. As ANN-based surrogate models significantly reduce computational time in comparison to traditional FE analysis, they are commonly incorporated in optimization frameworks. These models are routinely combined with genetic algorithms [40], gradient-based approaches [95] and other optimization techniques.

Deep physical informed neural networks (DPINN) have been used by Fang *et al.* [141] in the design of electromagnetic metamaterials who generated their designs by DPINN, focusing on improvements to the activation function as a route to circumventing high wave number problems. Deep neural networks as used to model all-dielectric metasurfaces can also be trained to predict performance at the atomic scale [144], which the researchers validated by comparing direct results against full-wave simulations using a commercial electromagnetic simulator. Magnusson and co-workers [143] use deep neural networks focused on improving the functionality of optical devices. In their work, they related the device outputs to the four parameters of the Stokes vector using a linear 4×4 matrix transformation. Deep neural networks were found to increase the number of outputs substantially over traditional algebraic methods that establish a correlation between input and output data. Chiroptical responses in 2D chiral metamaterials have been shown to benefit from deep learning (DL) approaches. When compared with traditional, rigorous coupled wave analysis (RCWA) methods for the study of circular dichroism (CD) in higher-order diffraction beams, DL is found to accelerate the design of hypersensitive photonic devices. Akashi *et al.* [142] compared Mie theory against neural network (NN) computations to solve scattering problems over the cross-section of a multi-layered cylinder (forward calculation). In their work, they report that the NN calculations were 3500 times faster than those based on Mie theory.

3.2.2 Inverse Design

The solving of inverse design problems is another major application area for ANN. It is well understood that the traditional forward design process can be time-consuming. In inverse design, a metamaterial structure needs to initially be suggested using intuition and insight, and in alignment with the performance requirements, as illustrated in Figure 9. The metamaterial structure is then analyzed, and further iterations or optimization steps are typically needed to further customize the structure. The design process is made more efficient when the relationship between the performance and design parameters is well established. The inverse design framework essentially analyzes the performance requirements and directly matches a metamaterial structure that perfectly suits the required specifications, by solving the problem inversely.

To build and train an ANN-based inverse framework, there has to be a solution for both forward design and the inverse problem. Some researchers choose to implement two separate ANN to deal with this task. In a publication by Kumar *et al.* [146] a multi-layer perceptron (MLP) architecture is used, with the first ANN mapping the design parameters onto the stiffness response of a spinodoid metamaterial in a forward fashion. This part of the framework serves as a surrogate model to replace FE analysis as described previously. The second, inverse ANN, is then trained using knowledge obtained from the surrogate model, to solve the inverse problem and relate stiffness requirements to the specific design parameters defining the metamaterial. As the inverse design approach significantly reduces both time and effort in the design process, it has gained popularity, for example, a similar approach employed by Ma

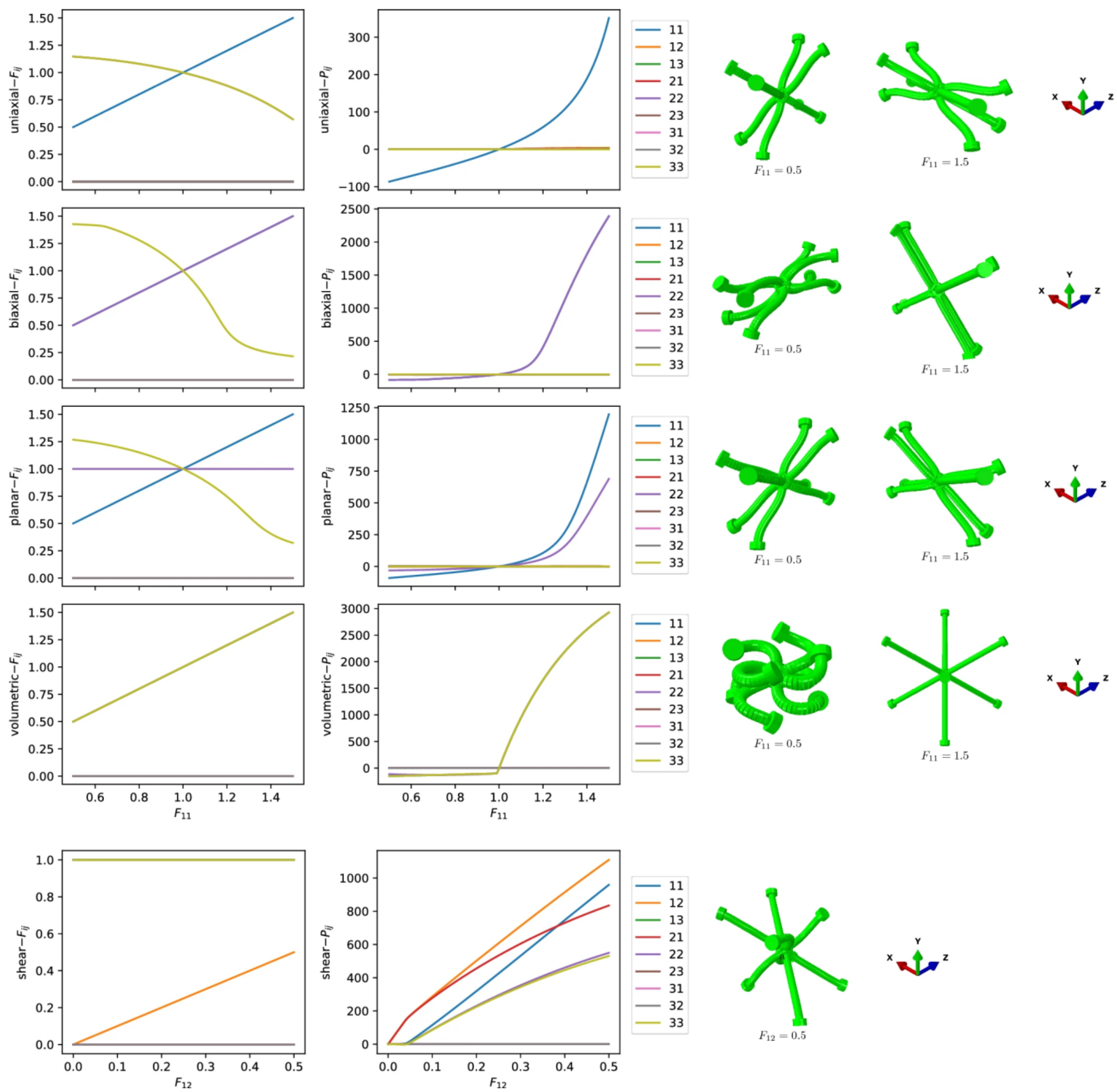

Figure 7: Training dataset of the X cell, showing all components of FF (left column of plots) and PP in Pa (right column of plots) for uniaxial, biaxial, planar, volumetric, and simple shear cases (from top to bottom). Reprinted with the permission of [137] under a Creative Commons CC-BY licence.

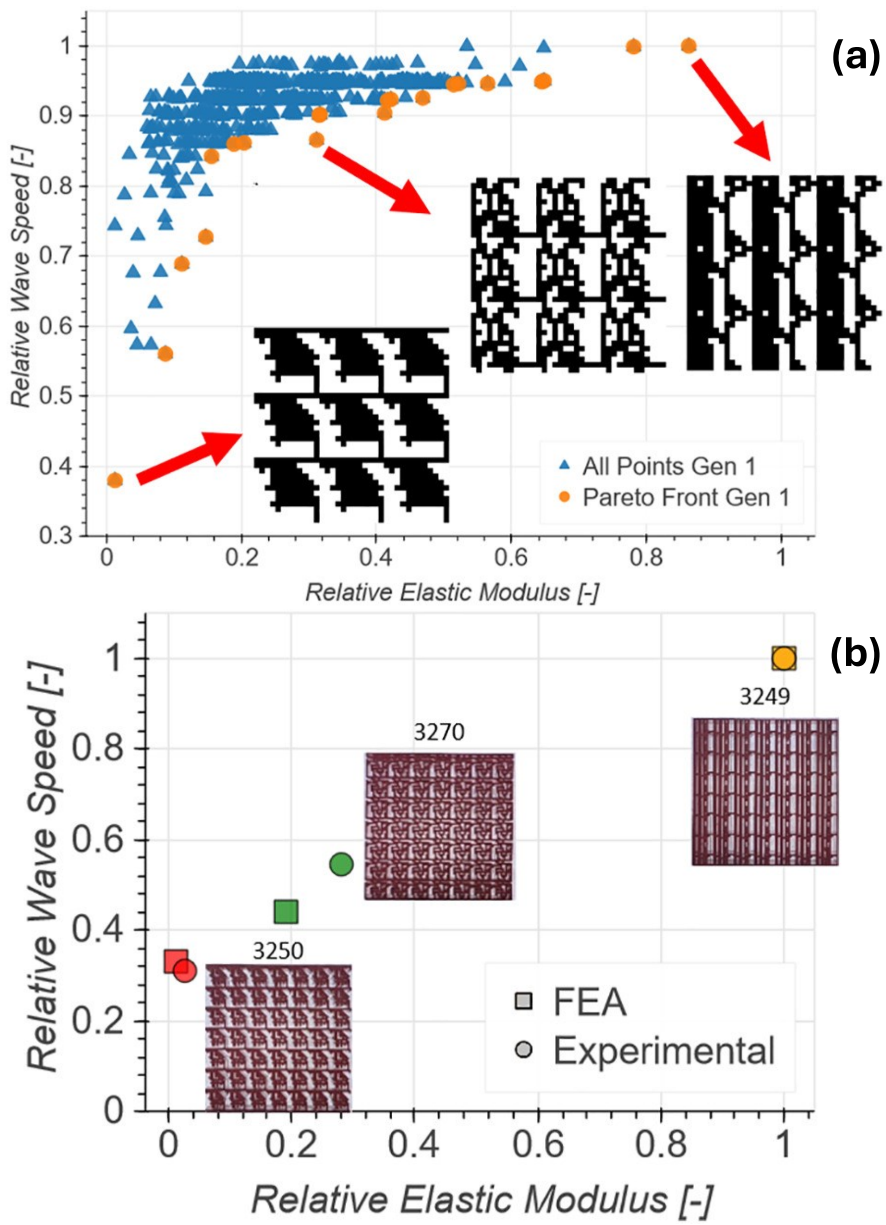

Figure 8: (a) Pareto front for the initial set of 1000 random designs, identified as generation 1. The axis values are normalized by the maximum value associated with 60% dense vertical columns and (b) normalised experimental results for the three generated designs compared to FEA results. Each design is given a different color. FEA data points are shown as squares, and Vero™ Magenta are shown as circles. Reprinted with the permission of [40] under a Creative Commons CC-BY licence.

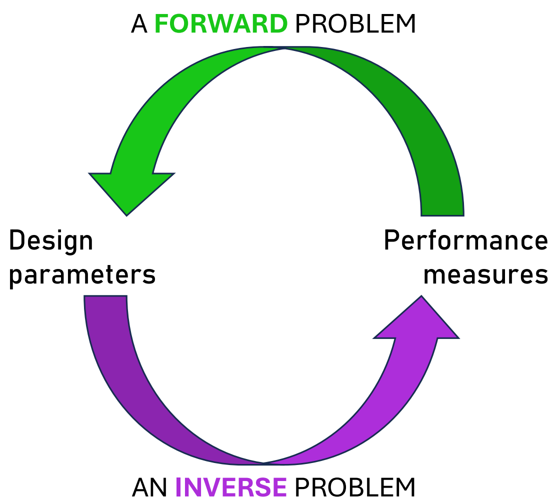

Figure 9: Forward and inverse problems in metamaterial design

et al. [105] focused on choosing 2D cellular structure patterns to match targeted force-displacement responses. The framework was able to predict the entire nonlinear response history, including large deformations within the plasticity region, rather than just a single mechanical property of the whole cell. Importantly, Ma and co-workers [105] elucidate that structure predictions made after only 20% of training reflect those at 100%, Figure 10. Since the inverse design approach has the ability to match the metamaterial structure to its full range of response, inverse design frameworks are gaining popularity for the prediction of full range spectral responses in photonic and plasmonic metamaterials. Hou *et al.* [147] demonstrated the use of ANN for on-demand design. A desired reflectance spectrum was provided as input to their framework, which consequently adjusted the parameters of a split ring resonator based nano-optic metasurface. Other research outputs show that similarly implemented frameworks used for the design of metamaterials match the required absorption [148], [149], circular dichroism (CD) spectra [150], [151], and scattering spectra [152]. Similar deep learning techniques have also been applied by some groups in the prediction of plasmonic [153] and photonic [109] properties in graphene-based metamaterials. A paper by Nanda *et al.* demonstrates a similar technique employing inverse ANN to design an electromagnetic split ring resonator based on metamaterial structures, relating design parameters with desired frequency and permeability values [108].

To ensure design suitability in some inverse problems, the range of admissible solutions may require the imposition of limits. In such cases, physics-informed neural networks (PINN) are useful as they solve learning tasks that need to respect the laws of physics, which are fundamentally solved through nonlinear partial differential equations. A paper by Fang *et al.* [141] and Chen *et al.* [154] demonstrated the usefulness of PINN in this respect, by using the method for the inverse design of cloaking metamaterials.

A number of researchers discuss the use of convolutional neural networks (CNN) in terms of their high suitability in image processing and analysis. CNN are mostly applied to metamaterial design processes when the structural or atomic arrangement is defined by a patterned image. Wilt *et al.* [155] used CNN to analyze pseudo-randomized Rorschach (ink blot) images and developed varying auxeticity metamaterials based on these patterns. Another example is from Liu *et al.* [156], who employed CNN architecture in meta-surface reflection phase predictions by analyzing planar patterns containing 16×16 square sub-blocks. Similarly, architectured networks have been utilized for mapping the geometrical properties of 2D frequency selective meta-surfaces and their corresponding reflectance and transmission spectrums [157]. In a paper by He *et al.* [158] CNN architectures were shown to be demonstrably useful for the analysis of spectral images when compared against processing the same type of information in a conventional data table format [148], [149]. The work elucidated inverse design processes of plasmonic metamaterial structures as also achievable by mapping their geometrical properties and optical responses.

With regards to autoencoder type architectures commonly used in dimensionality reduction tasks [120], [159], [160], a few papers report the exploitation of similar approaches for inverse design purposes. Harper *et al.* [161] explain many-to-one problems, discuss the limitations of traditional autoencoders, and propose a new pseudo-autodecoder (decoder-encoder architecture) that achieves high prediction accuracy. Their further work utilized the technique on broadband highly reflective meta-surfaces [110].

Generative networks (GN) are another class of the neural network framework that can be used in the discovery of new metamaterial structures. As the name suggests, GN are developed with the aim of generating new data, as opposed to the mapping of input-output relationships. In metamaterial design, applying GN enables a very broad exploration of the design space, much more so than in other ML techniques. This is because these frameworks are able to produce new structures that are not limited by the training set. The GN approach is therefore very suitable for the types of problems where the number of possible metamaterial structural arrangements is infinite, and the training data, no matter how large, is unable to capture all the possible variations. The two most commonly used in metamaterial related applications are variational autoencoders (VAE) and generative adversarial networks (GAN). VAE is a generative type neural network used in the inverse design of metamaterials. Similarly to traditional autoencoders, the network has an encoder part compressing the number of input variables into latent space, and another part with the objective of decoding the information in the most accurate way. VAE have an additional regularization term intro-

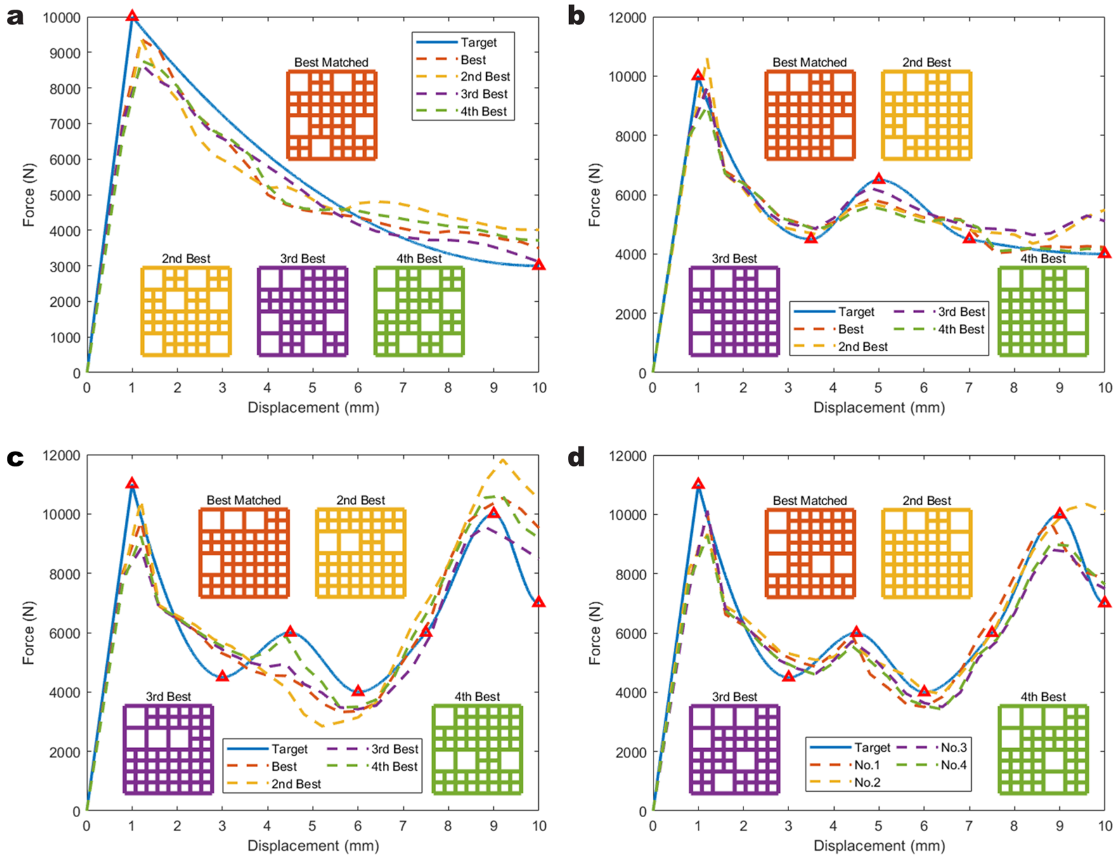

Figure 10: (a–c) Top four patterns and their reference curves for a targeted response with one, two and three load-dropping points only using the predicted responses by 20% training ratio. (d) Top four feasible patterns and their reference curves for the same target response in (c) using the reference responses of all available patterns. Reprinted with the permission of [105] under a Creative Commons CC-BY licence.

duced into the loss function of the autoencoder that ensures regularity within the latent space during training and helps to avoid data over-fitting. As a result, this ensures that the data within the latent space will have a sensible meaning once decoded, thus enabling a generative process using this network architecture. Liu *et al.* [162] use this technique for the inverse design of photonic nanostructures. They trained a VAE to reconstruct the input geometrical data of the metamaterial structures and then separate the decoder part to use it as a data generator. Randomly sampled vector values matching the distribution (check) of the latent space data were fed to the generator, which transformed the data to their corresponding structures. A similar approach was employed by Wang *et al.* [111] who used a VAE architecture to generate new 2D metamaterial structural assemblies that deform in a pre-programmed manner. The framework discussed in the publication is able to generate functionally graded metamaterials as well as heterogeneous structures that follow desired distortional behaviors. Distortional behavior has also recently been designed using combinations of biological structures [163], specifically leaf venation and trabecular bone. In their work, they used an unsupervised GAN to design novel metamaterial architectures with differing levels of structural hierarchy, showing thus that there is near infinite design potential for future metamaterial structures Figure 11. Lastly, Ma *et al.* [164] report on how VAE can be incorporated into a deep generative model for designing photonic metamaterials. A GAN usually has two separate neural networks that are trained simultaneously in an adversarial process. A generative part of the model produces a new metamaterial sample which is similar to those used in network training, while a discriminative part estimates the probability of the new sample coming from the generator rather than from the training set [165]. Throughout this competitive process, a GAN produces sets of completely new metamaterial structures that fall within the statistical distribution of the training set. A method of employing GAN for topology optimization has also been demonstrated by Kudyshev *et al.* [166] in their paper on meta-surface based thermophotovoltaics. The researchers created a GAN-assisted topology optimization framework by training the neural network using a set of topology-optimized designs. The design framework was shown to significantly reduce optimization time in comparison with direct optimization methods while generating high efficiency designs. Generative networks have also been shown as highly suitable for the discovery of new metasurfaces while solving inverse design problems [167]–[171]. In one of the earliest publications in the field [167], Liu and co-workers use a GAN architecture to conceptualize metasurface designs for optical applications that match user-defined optical spectra. After training was complete, the network was able to produce sets of previously unknown arbitrary patterns. This is in contrast to other ML practices, which fundamentally aim to optimize the geometrical parameters of the metasurface structure. The approach also ensures that local minima are avoided while the design space is explored, as multiple structures are generated for a single optical spectrum input.

3.2.3 Other ANN Applications

Optimization frameworks are usually parametric or topological when used to design metamaterial structures. Metaheuristic or gradient-based approaches are amongst the most commonly used for optimizations, however, many researchers also discuss approaches when optimization relies primarily on ANN.

Chen and co-workers [95] discuss a methodology using two ANNs in combination for the design of metamaterials. The first one called the 'predictor' acts as a surrogate model while the second one, the 'designer' is an optimization network that searches for the global minimum. It uses a backpropagation technique, which computes analytical gradients to find a solution to the optimization problem. In their findings, they note that although this gradient-based method might still get caught at a local minima, it is much faster than conventional numerical gradient-based approaches, such as finite-difference methods (FDM). Sarmah *et al.* [172] proposed the use of an ANN-based optimization framework, trained using several gradient descent algorithms. Their findings suggest that ANN is highly suitable for the optimization of design parameters and in their case for defining the performance of a split ring resonator. ANN have also been considered an alternative method for topology optimization. Kollmann *et al.* [173] used a CNN architecture to design 2D mechanical metamaterials by implementing a non-iterative topology optimization framework. In general, ANN is a data 'hungry' approach and sufficient data might be hard to obtain. This is especially true for more complex 3D meta-structures. Manufacturing or other design constraints might also limit the data that can be collected. Active learning may at times be a solution to this problem as the ANN trains while the other optimization cycle is running. Predictions at the beginning of this process are less accurate, however, they improve with each design iteration. Examples being active learning with GA [40] and learning with two ANN: a 'designer' and a 'predictor' [95] as discussed earlier in this paragraph. Calik *et al.* [174] discusses the optimization of ANN architecture and model parameters in more detail. The researchers use Bayesian optimization to enhance the performance of a deep learning based surrogate model replacing full-wave electromagnetic simulations. Their results suggest that a model developed using such methodology demonstrates a higher prediction accuracy and lower sensitivity to the variation in training samples in comparison to conventional and state-of-the-art regression methods. Harper *et al.* [175] also address the subject of optimal ANN design in metamaterial development. It employs Bayesian optimization with Gaussian processes to adjust the architecture and then the hyperparameters of the network mapping geometrical properties of all-dielectric metasurface structures to their reflective spectra. Their research focuses on the optimization of fully connected ANNs with one or two hidden layers and states the performance improvements. The findings suggest that similar optimization techniques can be applied to deeper networks such as CNN or GAN. There are also hy-

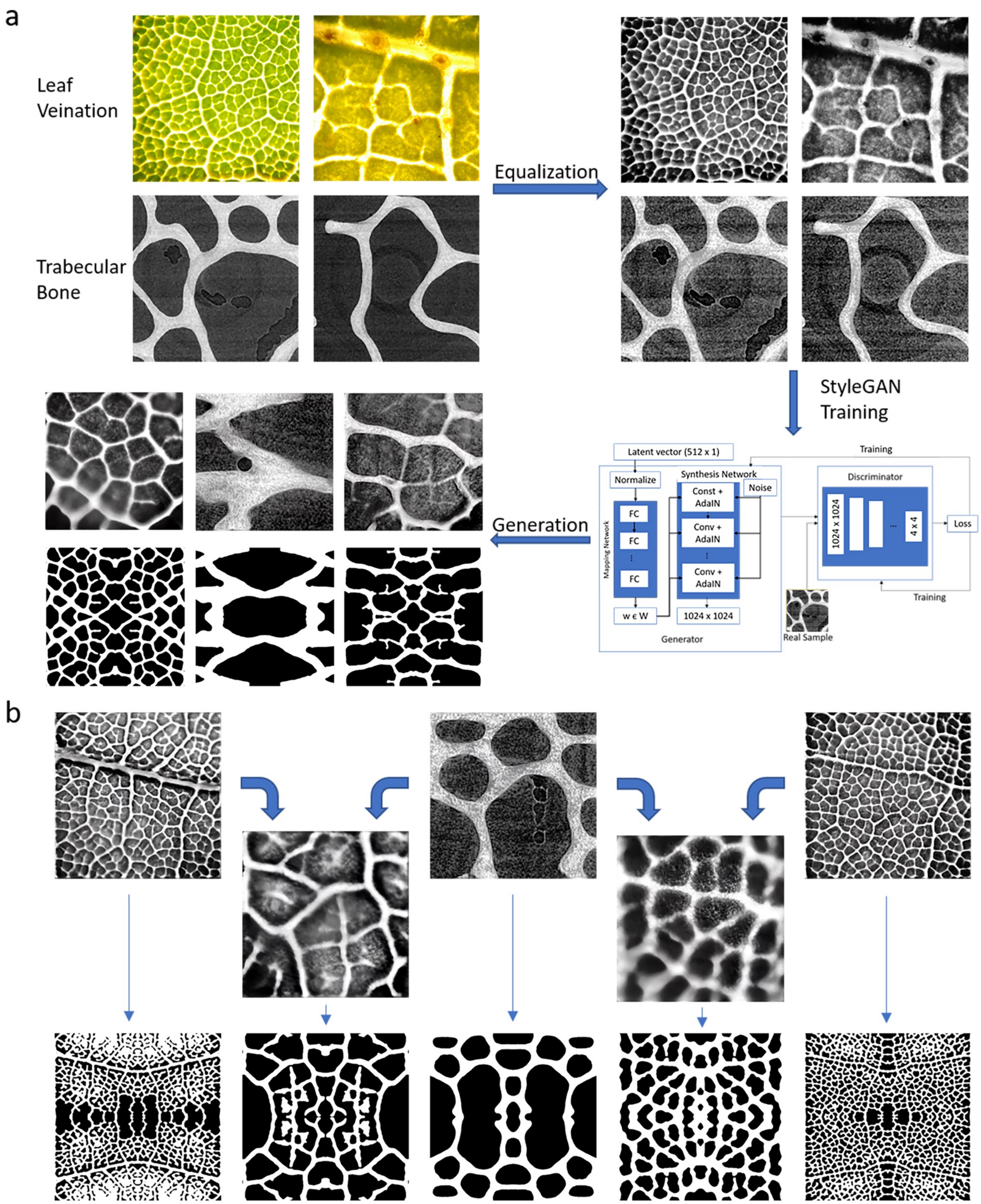

Figure 11: Unsupervised GAN for the combination of trabecular bone and leaf venation to create novel metamaterial structures. Reproduced with the permission of [163] under a Creative Commons (CC-BY) licence.

brid approaches where genetic algorithms (GA) and ANN are used in combination. [176] use this approach to develop a model predicting the chiroptical response of 2D diffractive chiral metamaterials. GA is used for finding the optimum number of neurons in each of the four hidden layers of the ANN. Similarly, Dong *et al.* [128] used GA in this hybrid approach to increase the predictive power of an ANN-based surrogate model for elastic metamaterials. Their results show that by adjusting the architecture and the hyperparameters of the network, the normalized mean absolute error (NMAE) was reduced from 1.1109 to 0.0278 in comparison to the results obtained from a finite element model. The final architecture contained 5 hidden layers with 19 neurons in each layer.

3.3 Nature-Inspired Algorithms in Metamaterials Design

Many nature inspired algorithms used in metamaterials design, are meta-heuristic approaches inspired by evolution, particle intelligence and physical processes. These algorithms exhibit stochastic behavior and iteratively explore design space using intelligent search strategies [177]. Meta-heuristic algorithms are typically adopted in optimization problems where there is a complex objective function landscape. They find global optima well and do not stagnate at local minima, as with certain other gradient-based approaches. These algorithms are also often applied to optimization problems with missing or imperfect information, which cannot be solved using other optimization techniques [178], for example, to optimize the geometrical arrangement of a metamaterial structure, to select the most suitable bulk materials from a database [179], or, to arrange a meta-atom assembly [180]. Meta-heuristic algorithms tend to find good or optimal solutions in a significantly shorter amount of time compared to brute force executive search methods. Hence, they are often used in design processes that have a considerable reliance on FEA or other computationally expensive metamaterial performance evaluation techniques. Nevertheless, meta-heuristic optimization algorithms are often considered computationally more expensive than other techniques. They have a tendency to find sub-optimal solutions, as finding precise positions of global maxima is impractical due to the additional computational costs involved. Most of these algorithms do not scale well with the increasing complexity of a design problem, and their suitability should be considered variable, depending on the extensiveness of available problem-specific information.

3.3.1 Genetic Algorithms

Evolutionary algorithms (EA), including but not limited to the genetic algorithms (GA) are a class of optimization algorithm that uses the individuals of a population as enablers to solutions in a given problem. These approaches work through genetic operators such as reproduction, mutation, recombination and selection. These operators develop solutions to problems by evolving the population. They are highly exploratory approaches and since each individual within a generation acts as an independent agent searching for the optimum, the computations can be executed in parallel. As with all meta-heuristic approaches, EA cannot ensure that the solution is optimal due to the nature of the random search, but they do find a near-optimal solution if it exists [181]. The literature suggests that although evolutionary algorithms take significant time to converge and are not the most efficient approach, they are robust methods and perform consistently well in all optimization problems [83]. GA algorithms can very efficiently elucidate minute geometrical alterations in mechanical metamaterials to maximize mechanical performance [10], [182] and recently Cerniauskas and Alam [183] revealed $> 4000\%$ improvements in specific shear properties were achievable from their base structures through GA regulated parametric optimization, Figure 12.

The most widely applied meta-heuristic search algorithms in metamaterial design are variations of the genetic algorithm. A few GA variants have been applied to design and optimize metamaterials. Simple GA algorithms for example, have been used to design inhomogeneous acoustic metamaterials by varying the coordinates in the Helmholtz equation [184], specifically, the team combined results from the theory of homogenization with GA. Importantly, they validated their outputs by designing different types of cloaks (curved rectangles, split rings and crosses) and after comparison against existing technologies, which their metamaterial designs mimicked well. Wu and co-workers [185] also made use of simple GA, but in their case to direct the assembly of phononic meta-atoms based metamaterials. Their work evidenced the possibility of GA use in modularizing metamaterials with both maximum and tunable bandgaps, by taking a bottom-up approach to design, starting at the scale of meta-atoms. Wang *et al.* [84] used a multi-island GA to parametrically optimize re-entrant auxetic honeycomb structures. The team analyzed the structures using a Python script based on Castigliano's theorem where mass was a constraint the Poisson's ratio was used to form the objection function. A non-sorting genetic algorithm (NSGA-2) discussed by Garland *et al.* [40] is an example of a multi-objective GA, which when combined with a surrogate CNN model was used to optimize the structures of lattice metamaterials. In their work, they noted that they could train the CNN more rapidly and with fewer example designs via active learning, a method that essentially allows the algorithm to select its own new training data. Another example of multi-objective GA is in [87] where tunable stiffness metamaterial structures in bone were optimized using NSGA-2. Here, the objectives were focused on tuning varied stiffness while minimizing von Mises stress. Design problems using GA often require lengthy computational times. To deal with this limitation, meta-heuristic searches can be combined with other techniques to exacerbate the process of metamaterial discovery. Luna *et al.* [86] for example, used GA with an ANN based surrogate model to reduce the computational time required for full wave numerical

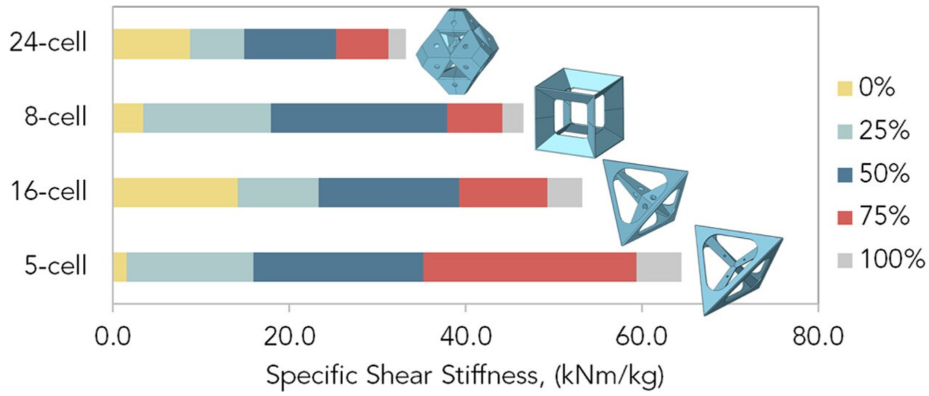

Figure 12: Specific shear stiffness comparison for 4-polytope projected mechanical metamaterial unit cells in shear at different levels of optimization with a 5-cell structure reaching $> 4000\%$ improvements in specific shear properties over its original unit cell structure. Reproduced with the permission of [183] under a Creative Commons (CC-BY) licence.

simulations in the design optimization of permittivity in electromagnetic metamaterials. It has further been shown that GA and ANN can be coupled for optimization and performance predictions in the development of modular mechanical metamaterials [185]. GA/ANN combinations have also been used in inverse design frameworks to generate a compositional pattern-producing network (CPPN) [3], which was used to compound meta-atoms into metallic metamolecules for the controlled design of optical metasurfaces. The team showed that even though metasurfaces typically have many intricate mechanisms as well as multiple degrees of freedom in view of design optimization, the rate at which these surfaces can reach an apical design is improved by CPPN. The design of dual polarizer metasurfaces was also optimized using an inverse design in combination with training through a deep learning network (DLN) serving as a forward model for GA, i.e. a deep learning forward genetic algorithm (DLF-GA) by Zhu *et al.* [186]. Here, the team focused on using the DLF-GA to predict the phase of meta-atoms for electromagnetic metasurfaces where dual (linear) polarization was specifically orthogonal. Other variations of GA such as micro genetic algorithms [187] have been applied as optimization methods for binary patterned nanostructures in tungsten based metasurface absorbers, and for developing inverse design frameworks with systematic arrangements such as mesh filters with grid patterns [188] of optical metamaterials.

Hybrid genetic program (HGP) is a tree based genetic program that generates random initial population designs for the purpose of both design synthesis and subsequent optimization. HGP uses user-defined cost functions to evaluate each individually generated design and the method has been shown to result in metamaterial based antennas with wider bandwidth absorbers than other nature inspired techniques [189]. A final extended GA technique, implemented for seismic metamaterials for the purpose of earthquake mitigation is Augmented Lagrangian Genetic Algorithm (ALGA) [190], which solves nonlinear optimization problems that have a combination of linear and nonlinear constraints, and bounds and is an algorithm integrated within popular commercial modeling tools such as Matlab.

3.3.2 Particle Swarm Intelligence Algorithms

Ant Colony Optimization (ACO) is inspired by the foraging behavior of ants. It recreates a population of artificial ants that deposit pheromones on paths as they explore a solution space. Over time, paths with higher pheromone levels become more attractive, leading to the discovery of optimal or near-optimal solutions as evidenced from some of the earlier papers in this area [191], [192], which primarily consider electromagnetic metamaterial antennae and the prediction of bandwidth. ACO is often also used for combinatorial optimization problems [89]. Alharbi *et al.* for example recently proposed a Dipper-Throated (DT) optimization for ACO (DTACO) [193] as a viable method for predicting the bandwidth of electromagnetic metamaterials, which in turn is an enabler for the manipulation of bending, absorbing or amplification of electromagnetic waves. DT optimization is essentially one that assumes birds fly and swim to find food and the optimization takes into account bird numbers, velocities, and positions. The researchers note that though the method is reliable, its reliability requires accurate models and simulations of the metamaterials under consideration, and that without accurate initial models, the method provides inaccurate predictions of bandwidth. The spatial filtering of electromagnetic waves is important when designing metamaterials that are frequency selective surfaces (FSS). While much of the work in this area is dealt with in 2D, Zhu *et al.* [194], [195] used a multi-objective lazy ACO (MOLACO) to consider both polarization problems and angle independent design in 3D FSS, generating unintuitive structures based on wire grid resolutions that superior to conventional planar, multilayer and 3D FSS in terms of angular performance and unlike traditional designs, were not polarization dependent.

Particle Swarm Optimization (PSO) is another effective optimization method of the geometrical parameters in metamaterials. It can be used to fine-tune the shape, size, and arrangement of metamaterial elements to achieve specific optical, acoustic, or thermal properties. PSO is also applied in designing cloaking devices using metamaterials such as antennas [90] [196]. Choudhury *et al.* [197] developed PSO to yield structural parameters in metamaterials relevant at specific resonant frequencies. The team optimized square split ring resonator (SRR) metamaterials and noted that the increase in resonant frequency, was due to the square micro-sized split in the SRR, and that post-PSO optimization, the SRR showed improved directivity. Similar conceptual benefits are reported for circular patch split structures [198]. There has been some work focused on combining PSO with neural network (NN) methods to improve predictive capacity. Zhang *et al.* [199] for example, combined CNN and binary particle swarm optimization (BPSO) to alter the reflection phases of metasurfaces to match a desired target. BPSO algorithms have also been discussed [200] in terms of topology optimization for the 3D design of negative permeability dielectric metamaterials. Here, the researchers compared the PSO optimized topologies against those modeled using the commercial FEA tool ANSYS. After comparison, while FEA was found to yield accurate results, the CPU time was significant as compared to the PSO, the main benefit of which over FEA was computational time saved. Song *et al.* [201] provide another example, this time combining ANN and PSO. They used a radial basis function neural network RBF-NN as a surrogate between geometric parameters and predicted frequency responses in electromagnetic metamaterial absorber structures.

Bee Colony Optimization (BCO) algorithms have, albeit to a lesser degree than PSO and ACO, been used to optimize metamaterials in various applications, including microwave absorbers, lenses, and beam steering devices. Artificial bees can be used to explore the design space and adapt the properties of the metamaterial to reach specific target requirements [91]. Gaynutdinov *et al.* [202] used a BCO technique to optimally parameterize metamaterials to generate an electromagnetic shield with operator specified coefficients for reflection and transmission. Yu *et al.* [203] used BCO to accelerate the rate at which permittivity and thickness of wire metamaterials for use as resonant cavity antennas, could be determined. The optimization of magneto-mechanical metamaterials structures has received recent attention from Ma *et al.* [204], who used a discrete artificial bee colony to find optimal structure-distributions within these metamaterials for targeted strains. The authors trained a ResNet to replace FEA based outputs, thus significantly decreasing optimization output times.

Firefly Algorithms (FA) can be applied to optimize the light manipulation properties of metamaterials, for example by creating metamaterials with unique refractive indices, or, light-focusing capabilities. Fireflies adjust the parameters of metamaterial elements to achieve desired optical effects [92]. While they are not as popular as ACO and BCO, there are several instances where FA have found usefulness as a tool within the design process for, especially, electromagnetic metamaterials. Using FA, Saraswat [205] developed a hybrid fractal SRR metamaterial antenna for multiband operations such that the design contributed to resonance between 1.9-15.2GHz. In their earlier work Saraswat and Kumar [206] had also considered miniaturization methods for SRR metamaterials in quad based antennas. While FA is known to be a generally efficient and speedy algorithm that is concurrently easy to implement [207], it can experience convergence problems through entrapment in local minima, with FA control parameters being a randomization parameter and an absorption coefficient. To counter FA convergence problems and thus improve the effectiveness of FA, Srivastava *et al.* [208] incorporated an inertial weighting within the FA to balance trade offs between local and global FA searches, and consequently also improving the precision and accuracy of fraction delay filter designs, which has relevance in antenna engineering.

Cuckoo Search (CS) algorithms have been used to enable the optimization of structural parameters in metamaterials to improve specific electromagnetic or acoustic properties. Cuckoos can lay eggs (representing candidate designs) in nests (representing solutions) to explore and improve the design space [93]. Examples of CS in metamaterials design include the work of Yang *et al.* [209] whose focus was on acoustic metamaterials with multiple parallel hexagonal Helmholtz resonators, more recently researched by [210], Yang *et al.* [211] whose work focused on the structural parameterization of metamaterials for sound absorption, and the development of thin multi-layer metamaterial sound absorbers through CS based parameter optimization [212].

4 Discussion

4.1 General Trends

Our analyses reveal that the most popular techniques, by the number of publications, are evolutionary algorithms and artificial neural networks. A summary of methods is provided in four separate tables in the Appendix, focusing on ANN (Appendix Table 1), ML excluding ANN (Appendix Table 2), nature inspired AI (Appendix Table 3), and combined methods (Appendix Table 4). Approximately half of all publications we reviewed use a variation of an evolutionary algorithm while a little under half relied on a neural network. Less than 10% of the papers used different approaches of AI and ML such as gradient-based methods and dimensionality reduction techniques. Figure 13 shows the percentage share of different methodologies used over the last five years. This pie chart reflects the rapid increase in the preferred use of ANN for metamaterial applications. The dominant application areas of the two techniques differ and the techniques are not mutually exclusive. Whilst ANN is used for mainly 3 specific applications namely, inverse design, surrogate modeling and hyperparameter optimization, GA and its derivatives have a wider range of applications. They are primarily for optimization such as parameter optimization and inverse design. Additionally, there are several publications we discussed that use hybrid approaches, combining the strengths of different AI techniques. We are now in a position to extend Figure 3 in a way that allows us to identify more specifically the AI areas applied to metamaterials design and engineering, Figure 14. While in this new figure we note that the exponentially increasing trend is still evident as was notably the case in Figure 3, we also note high surges in recent years in the NN, ML and EA histogram bars, with significant increases also noticeable with GA. Currently, ML algorithms are clearly very popular and ultimately, each approach exacerbates the rate of discovery of new metamaterial architectures, which is indubitably the reason these AI methods have gained so much popularity. The main areas of AI application in the metamaterials design space are summarized in the pie chart of Figure 15. Here, we note that mechanical metamaterials are the largest application area, followed by areas related to the manipulation of light-based waves i.e. biosensor-based, photonic, plasmonic, acoustic, electromagnetic, etc.

4.2 Opportunities and Challenges

Our review conveys the importance that artificial intelligence (AI) has in metamaterial design in modern times. AI enables the exploration of a broad range of possible new materials discoveries. The integration of AI has already led to several breakthrough discoveries in material science and engineering. Some of the key advantages and challenges of machine intelligence in metamaterials design as indicated by our review follow.

4.2.1 Efficient Exploration of Design Space

AI algorithms, such as genetic algorithms, neural networks, and reinforcement learning, can efficiently explore complex metamaterial design spaces to find novel and optimal structures, saving time and resources compared to brute force algorithms, analytical methods, or iterative trial-and-error methods. Time efficiency means informed decision-making is easier at the user-level [213], and the recognition of specific performance criteria can reduce the need for extensive testing, whether experimental or virtual [214]. In addition, complex patterns and relationships within the available data can be analyzed, as part of the fundamental design process. Existing material properties can also be analyzed and patterns suggested leading to desirable behaviors and properties. Vast design spaces can be explored with a high degree of precision and detail that would be impractical or impossible for human designers [215]–[217].

4.2.2 Multi-Objective Optimization

Machine learning models like neural networks, can be trained to model the relationships between specified design parameters and a range of different material properties [218], [219]. These models approximate complex, nonlinear objective functions, enabling efficient optimization from baseline input structures. Genetic algorithms (GA) and particle swarm optimization (PSO) explore this by iteratively generating and evaluating designs. Convergence towards Pareto-optimal solutions [220], [221] can further the efficient exploration of the vast metamaterials design space by generating candidate designs based on prior knowledge and simulations. Reinforcement learning algorithms, for example, can learn optimal strategies for exploration, rather than solely focusing on performing architectural optimizations [222]. AI can also create surrogate models of complex simulations, which are otherwise computationally expensive. Surrogate models, such as Gaussian processes [223], approximate the simulation results, allowing for faster iterations during the process of optimization.

4.2.3 Materials Discovery

AI as discussed in this review, is seen to accelerate the discovery of new materials by predicting their properties. This can be conducted at varying length scales, from the atomic-level to the macro-scale. Atomic-level design decisions leading to novel and unique atomic arrangements result in a knock-on effect at the macroscopic level [180], affecting macro-scale metamaterial properties and behaviors. Machine learning algorithms and neural networks (CNN, GAN, CGAN), furthermore, can be used to analyze broad datasets of materials properties and their atomic structures. By identifying patterns and correlations within the data, the properties of new metamaterials based on their composition, structure, and other factors [72] [73] [77] can be predicted. Genetic algorithms and evolutionary optimization techniques generate and evolve candidate materials by iteratively modifying their compositions or structures to improve specified properties. As such, it is clear that AI enables the discovery of new materials that may not otherwise have been considered using traditional methods [184] [185]. By analyzing a broad range of candidate compositions and structures, these techniques create unconventional metamaterials with potentially unique properties and behaviors.

4.2.4 Data Availability and Quality

Through our review, we noted that the availability and quality of data are two significant challenges when AI techniques are applied to metamaterial design. This is especially true in data-driven models, which require large, high-quality datasets [224]. Metamaterial design often involves high-dimensional data, making it challenging to collect, store, and analyze the relevant information effectively. Obtaining comprehensive and reliable data on materials properties and their corresponding structures can be challenging, particularly in the case of emerging materials. Some metamaterial properties or structures may also be unconventional, leading to sparse data points within the design space. Sparse data can make it difficult for AI models to generalize effectively [225]. Moreover, gathering unique experimental data is expensive and time-consuming,

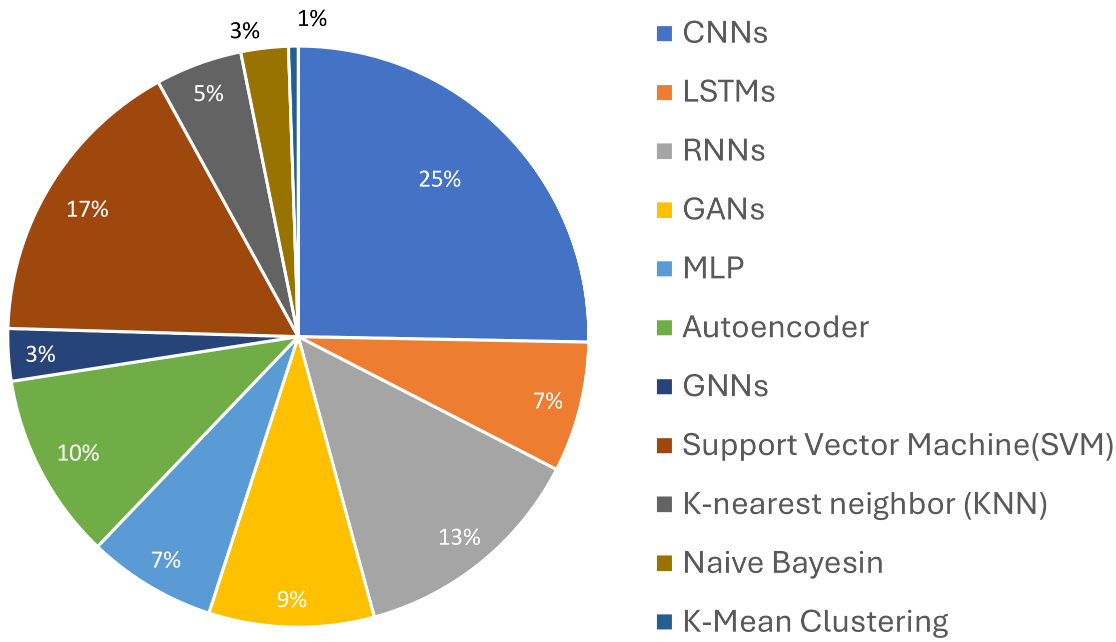

Figure 13: Publications categorized by machine learning algorithms used in metamaterials design. CNN - convolutional neural network, LSTM - long short-term memory, RNN - recurrentneural network, GAN - generative adversarial network, MLP - multilayer perceptron, GNN - graph neural network.

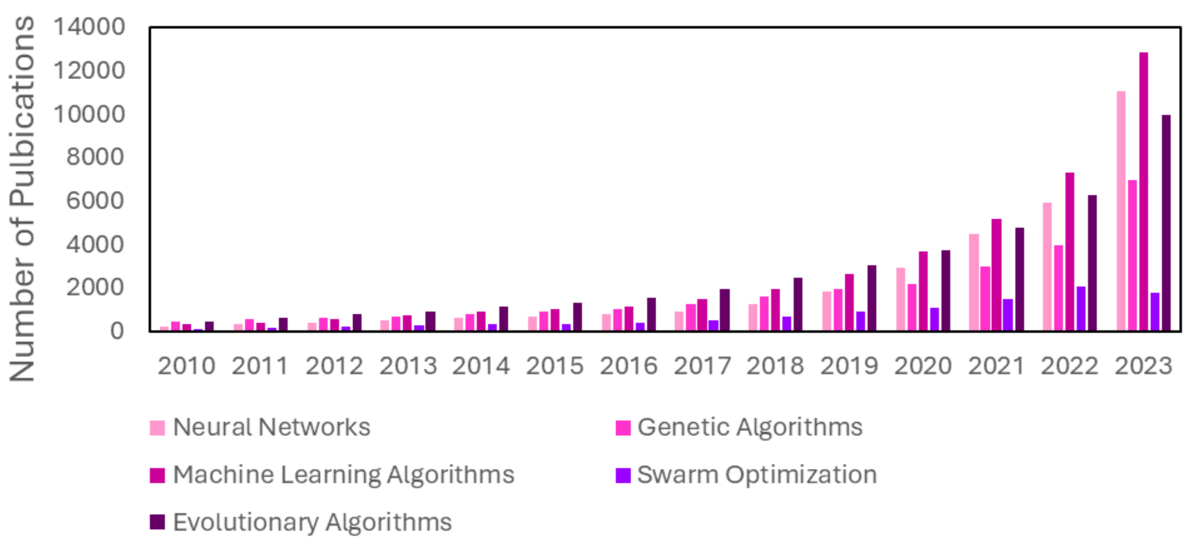

Figure 14: Increasing trend of different AI-based and nature-inspired techniques in metamaterials.

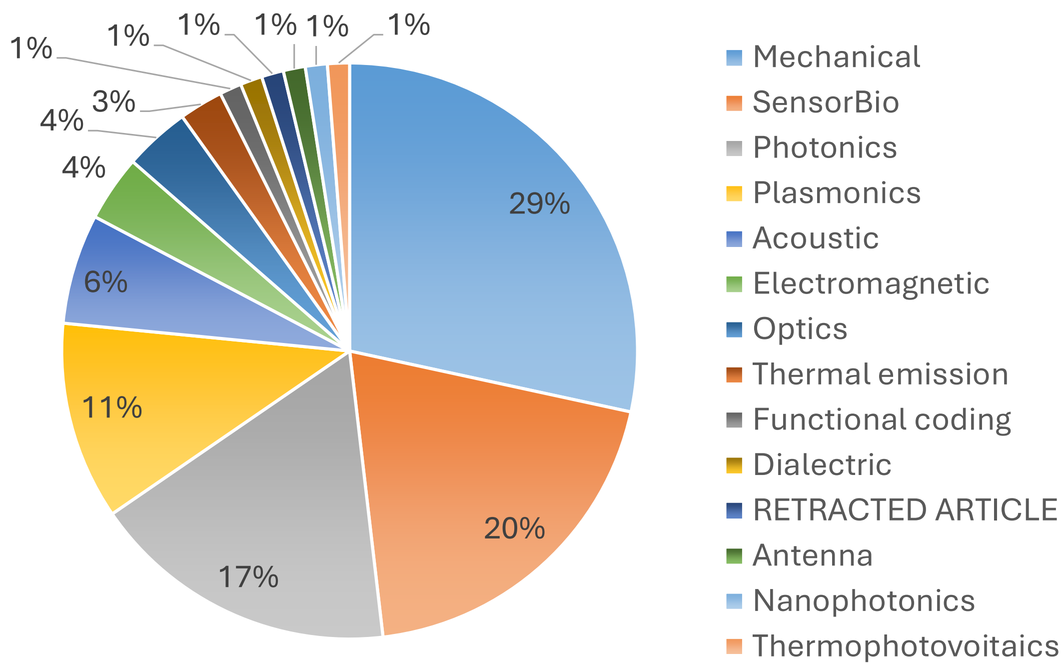

Figure 15: Publications categorized by application area

thus limiting the quantity and variety of data that can be available for training and validation.

4.2.5 Computational Resources

Training complex AI models, in particular deep learning models, are computationally intensive and powerful hardware may be needed to ensure that the full benefit of the AI is achieved. When it comes to metamaterials, a further challenge arises due to the complex nature of their design problems, which involve high-dimensional design spaces, intricate simulations, and computationally expensive optimization processes [226]. Metamaterial design tasks frequently require parallelization with numerical simulations to evaluate the performance of candidate designs in real time. Such simulations are computationally and resource expensive and are also time-consuming.

4.2.6 Interdisciplinary Expertise

Effective metamaterial design requires collaboration between materials scientists, physicists, engineers, and AI programmers [227]. Choosing the appropriate AI optimization algorithm is challenging, as different algorithms perform differently depending on the problem. Researchers must carefully select the most suitable algorithm for a specific metamaterial design task. AI approaches optimize designs based solely on data-driven patterns, without a deep understanding of the underlying metamaterial physics or materials science, leading often to unconventional or counter-intuitive designs that can be difficult to interpret. Bridging the gap between these disciplines and integrating the knowledge is a challenge that has to be overcome for the design process to itself reach an optimum [228].

4.2.7 Robustness and Generalization

AI models must be robust and capable of generalizing well beyond the training data. Since metamaterials are inherently complex, often exhibiting nonlinear behaviors [229]–[231], it can be challenging to create models that are sufficiently effective at generalization. Metamaterials behave differently under different conditions (temperature, pressure, humidity, etc.), and as such, the collection of data to circumvent specific variability is challenging and can lead to uncertainty in the predictions made. Moreover, models may memorize the training data [232], instead of learning from underlying principles, which itself can result in poorer levels of generalization.

4.2.8 The Causal Relationship Problem

Our review reveals that traditional ML does not consider causal relationships between variables and as such does not lead to direct solutions [233]. Many widely used neural network (NN) models, such as deep learning models, are often referred to as ‘black boxes’ because they lack transparency and interpretation [234]. They can make accurate predictions or classifications, but the challenge is then to understand how specific decisions have been made, and to subsequently explain the causal relationships between inputs and outputs. Deep neural networks, especially with complex architectures, can capture extremely complex patterns and relationships in data [235], [236]. While this is beneficial for prediction accuracy, it can make it very difficult to interpret the reasons underlying particular decisions. Due to high non-linearity in ANN models, small changes in input features can lead to large, unintuitive variations in the model output, making it hard to understand cause-effect relationships.

4.2.9 Hyperparameter Optimization and Hybrid ANN & GA

Although the literature suggests that AI-based surrogate modeling is often used in developing metamaterials, the common issue remains the selection of hyperparameters [237] (e.g. batch sizes, activation and loss functions) and model architecture (e.g. shape of the network, number of nodes and layers). Hyperparameters are values that control the learning or optimization process. As is widely known, the selection of hyperparameters is a key factor that determines both the quality of the outputs and the performance of the algorithms. This applies to both nature-inspired [204] and ML algorithms [238]. Experience and intuition-driven model setups typically rely on trial-and-error based approaches which can lead to sub-optimal performance.

4.3 Future Perspectives

We anticipate that the use of artificial neural networks in metamaterial discovery frameworks will continue to grow based on evidence on the current growth rate of the number of publications per year (cf. Figures 3 and 14). AI approaches in metamaterial design hold significant promise in revolutionizing the field and unlocking new capacities for designing and engineering metamaterials [239] with unique properties and behaviors. Since machine intelligence is both customizable and flexible [43], we anticipate high predictive power ANN-based models will be used alongside inverse design frameworks, mapping thence, metamaterial performance to their parameters and further accelerating the discovery of novel metamaterials. Generative models and reinforcement learning will expedite the discovery of new metamaterials [240], accounting for uncertainties in material properties and in fabrication processes. Moreover, as computational power continues to rise, the rate of machine intelligence based metamaterials discoveries will rise. AI will play a crucial role in solving complex inverse design problems, where the desired properties are specified, and machine intelligence will search for and find the relevant structures to meet the specifications. In terms of data-driven design, AI techniques, including machine learning and data analytics, will leverage progressively larger materials properties datasets and over time, as the body of experimental material properties data expands, more explicably accurate designs will emerge [241], [242]. AI will be integrated into additive manufacturing and nanofabrication as design optimization will need to take into account limitations in manufacturing. The integration of machine intelligence into architectural design concurrent with manufacturing parameterization will enable a rapid realization of complex structures that can also be made efficiently and at speed [243]. Greater interdisciplinarity and collaboration will be needed with experts from a variety of fields interacting to fine-tune discipline specific concepts into the design process.

Evolutionary Algorithms (EA) are extremely powerful [244] and remain the most commonly used technique since they can optimize models when information is incomplete or only partially available. The hybridization of AI techniques is increasing, with primary combinations at present being machine learning and deep learning. Hybridization can enhance the effectiveness of EA by integrating data-driven insights, predictive models, and optimization. EA will become more proficient at handling constraints, including physical, manufacturing, or structural constraints, to ensure that the designed metamaterials meet specifications. To reduce the computational cost of evaluating metamaterial designs, EA will increasingly rely on surrogate models [97], [128], such as Gaussian processes or neural networks, as they approximate objective functions. This will in turn accelerate the optimization process [245], [246]. In summary, both Artificial Intelligence (AI) and Evolutionary algorithms (EA), including machine learning, are powerful tools in metamaterials design. While AI with machine learning encompasses a broader range of techniques and methods, EA have their own unique strengths and applications [198], [247], [248]. The future of EA in metamaterial design is shaped by their distinct characteristics and specific challenges. AI offers powerful gradient-based optimization methods and data-driven insights for metamaterial design. EA remain valuable tools for global optimization, handling complex design spaces, and addressing challenges with noisy or expensive objective functions. The future likely involves greater synergy between both approaches to unlock more potential within the metamaterials design space.

Mechanical metamaterials as previously discussed in Figure 15, are the largest specialized area where machine intelligence is used for design optimization. In this branch of metamaterials, the two main directions of research are performance prediction and inverse design. Since mechanical metamaterials exhibit by default, a hierarchy in design for properties, machine intelligence will need to look beyond specifically performance prediction and inverse design, as other aspects such as manufacturing constraints [183], microstructural design for macroscopic properties, and the optimization of operation controls [249]. An emergent branch of mechanical metamaterials is, 'unfolding structures'. These are often large deformation structures typically designed to fold from flat sheets into 3D structures, taking inspiration from arts such as origami and kirigami [250]. While origami and kirigami metamaterials are receiving increasing attention [251]–[254], the utility of machine intelligence in their design and construction is still low compared to unit-cell based structures. Many papers in this area consider topology and unit cell arrangement for controlled deformation [255]–[258], and the total percentage of papers using machine intelligence in conjunction with origami or kirigami metamaterials is $< 2\%$ overall, and in 2023, the percentage has dropped further to $< 1.5\%$. This is probably partly due to the popularity of unit-cell based metamaterials, but we presume that the rate of growth of machine intelligence in origami/kirigami metamaterials design will increase over time and that this will likely be a result of the development of more generalized AI methods.

The future of machine intelligence in metamaterial design is an exciting frontier. With time, it will be integrated into all levels of technology readiness, becoming commonplace as an assistive tool in the computational design of metamaterials.

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Conflicts of Interest

The authors declare no conflicts of interest.

Author Contributions

Conceptualization (GC, PA); Data curation (GC, HS, PA); Formal analysis (GC, HS, PA); Funding acquisition (HS, PA); Investigation (GC, HS, PA); Methodology (GC, HS, PA); Project administration (PA); Resources (HS, PA); Software (GC, HS, PA); Supervision (PA); Validation (GC, HS, PA); Visualisation (PA); Roles/Writing - original draft (GC, HS, PA); Writing - review and editing (GC, HS, PA).

Appendix

Table 1: Table summarizing papers that use ANN in metamaterials design.

	Publication	Year	Method(s)	Application of AI
	Application field: Acoustic			
1	Ma, Cheng, and Liu [259]	2018	Deep Learning	Optimization framework
2	Xu, Guan, Bao, *et al.* [260]	2018	CNN	Optimization framework
3	White, Arrighi, Kudo, *et al.* [246]	2019	ANN	surrogate Model
4	Robeck, Cipolla, and Kelly [261]	2019	CNN	Optimization framework
5	Hughes, Williamson, Minkov, *et al.* [262]	2019	ANN	Inverse design
6	Sajedian, Kim, and Rho [263]	2019	CNN, RNN	Optimization framework
7	Bostanabad, Chan, Wang, *et al.* [264]	2019	ANN	Inverse Design
8	Wu, Liu, Wang, *et al.* [265]	2020	ANN	Inverse Design
9	Weng, Ding, Hu, *et al.* [266]	2020	Deep Learning	Classification
10	Melo Filho, Angeli, Ophem, *et al.* [267]	2020	ANN	Inverse Design
11	Chen, Lu, Karniadakis, *et al.* [268]	2020	Deep Learning	Inverse Design
12	Kollmann, Abueidda, Koric, *et al.* [269]	2020	Deep Learning	Optimization Framework
13	Qu, Zhu, Shen, *et al.* [270]	2020	ANN	Optimization Framework
14	Lai, Amirkulova, and Gerstoft [271]	2021	CNN, GAN	Inverse Design
15	Gurbuz, Kronowetter, Dietz, *et al.* [272]	2021	GAN	Inverse Design
16	Amirkulova, Tran, and Khatami [273]	2021	Deep Learning	Inverse Design
17	Wu, Liu, Jahanshahi, *et al.* [274]	2021	ANN	Inverse Design
18	Shah, Zhuo, Lai, *et al.* [275]	2021	RL	Optimization Framework
19	Tran, Amirkulova, and Khatami [276]	2022	ANN	Inverse Design
20	Wiest, Seepersad, and Haberman [277]	2022	GNN	Inverse Design
21	Amirkulova, Zhou, Abbas, *et al.* [278]	2022	Deep Learning	Inverse Design
22	Tran, Khatami, and Amirkulova [279]	2022	CNN	Inverse Design
23	Li, Chen, Li, *et al.* [280]	2023	CNN	Inverse Design
24	Li, Chen, Li, *et al.* [281]	2023	Deep Learning	Inverse Design
25	Wang, Chen, Xu, *et al.* [282]	2023	ANN	Inverse Design
	Application field: Electromagnetics			
26	Jiang, Xiao, Liu, *et al.* [283]	2010	ANN and scaled conjugate gradient	Surrogate model
27	Freitas, Rêgo, and Vasconcelos [140]	2011	ANN	Surrogate model
28	Vasconcelos, Rêgo, and Cruz [139]	2012	ANN	Surrogate model
29	Sarmah, Sarma, and Baruah [172]	2015	ANN	optimization framework
30	Saha and Maity [138]	2016	ANN	Surrogate model
31	Nanda, Sahu, and Mishra [108]	2019	ANN	Inverse design
32	An, Fowler, Shalaginov, *et al.* [144]	2019	ANN	Surrogate model
33	Yuze, Hai, and Qinglin [157]	2019	CNN	Classification and clustering
34	Liu, Zhang, and Cui [156]	2019	CNN	optimization framework
35	Hodge, Mishra, and Zaghloul [284]	2019	DC-GAN	Inverse design
36	Hodge, Mishra, and Zaghloul [169]	2019	DC-GAN	Inverse design
37	Hodge, Vijay Mishra, and Zaghloul [170]	2019	DC-GAN	Inverse design
38	Kudyshev, Kildishev, Shalaev, *et al.* [166]	2019	DC-GAN	Topology optimization
39	Fang and Zhan [285]	2020	ANN (Deep physical informed neural network)	Surrogate model
40	Khatib, Ren, Malof, *et al.* [286]	2021	ANN(Deep Learning)	Inverse design
42	Zhu, Qiu, Wang, *et al.* [287]	2021	Transfer Learning	Inverse design
43	Xu, Luo, Luo, *et al.* [288]	2021	Transfer Learning	Inverse design
44	Zhang, Qian, Fan, *et al.* [289]	2022	Transfer Learning	Inverse design
45	Trinh, Guilleminot, Perrot, *et al.* [290]	2022	Transfer Learning	Inverse design
46	Aybike and KİLİMCİ [291]	2021	CNN	Inverse design
47	Zhou, Qiu, Zhang, *et al.* [292]	2022	ANN	Optimization framework
48	Zhou, Xiao, and Wang [293]	2022	Deep Learning	Inverse design
49	Fantoni, Bacigalupo, Gnecco, *et al.* [294]	2023	Deep Learning	Inverse design
50	Khatib, Ren, Malof, *et al.* [295]	2023	Deep Learning	Optimization framework
	Application field: Mechanical			

Continuation of Table 1

	Publication	Year	Method(s)	Application of AI
51	Gu, Chen, Richmond, *et al.* [134]	2018	CNN	Surrogate model
52	Kumar, Tan, Zheng, *et al.* [146]	2020	ANN	Inverse design
53	Ma, Zhang, Luce, *et al.* [105]	2020	ANN	Inverse design
54	Xue, Beatson, Chiaramonte, *et al.* [136]	2020	ANN	Surrogate model
55	Wilt, Yang, and Gu [107]	2020	CNN	Inverse design
56	Kollmann, Abueidda, Koric, *et al.* [173]	2020	CNN	Topology optimization
57	Fernández, Jamshidian, Böhlke, *et al.* [137]	2021	ANN	Surrogate model
58	Whalen and Mueller [245]	2021	Transfer Learning	Inverse design
59	Wang, Zhuang, Xian, *et al.* [296]	2021	Transfer Learning	surrogate Modeling
60	Shah, Zhuo, Lai, *et al.* [297]	2021	Reinforcement Learning	Inverse design
61	Kim, Kim, Yang, *et al.* [298]	2022	Transfer Learning	Optimization framework
62	Wang, Zhuang, Xian, *et al.* [299]	2022	Transfer Learning	surrogate Modeling
63	Wang, Zeng, Wang, *et al.* [300]	2022	Genetic Algorithms	Inverse design
64	Mastrigt, Dijkstra, Hecke, *et al.* [301]	2022	CNN	Classification
65	Mastrigt, Dijkstra, Hecke, *et al.* [301]	2022	ANN(Deep Learning)	Rational design
66	Zeng, Zhao, Lei, *et al.* [302]	2023	ANN(Deep Learning)	Inverse design
67	Zeng, Zhao, Lei, *et al.* [303]	2022	ANN(Deep Learning)	Inverse design
	Application field: Optics			
68	Ma, Cheng, and Liu [149]	2018	ANN	Inverse design
69	Magnusson, Mueller, Juhl, *et al.* [304]	2018	ANN	Surrogate model
70	Liu, Zhu, Rodrigues, *et al.* [305]	2018	DC-GAN	Inverse design
71	He, He, Zheng, *et al.* [158]	2019	ANN	Inverse design
72	An, Fowler, Zheng, *et al.* [151]	2019	ANN	Inverse design
73	So, Mun, and Rho [150]	2019	ANN	Inverse design
74	Chen, Zhu, Xie, *et al.* [109]	2019	ANN	Inverse design
75	Akashi, Toma, and Kajikawa [306]	2019	ANN	Surrogate model
76	Ma, Cheng, Xu, *et al.* [164]	2019	GAN	Inverse design
77	Harper, Weber, and Mills [307]	2019	Pseudo autoencoder	Inverse design
78	Ashalley, Acheampong, Besteir, *et al.* [148]	2020	ANN	Inverse design
79	Hou, Tang, Shen, *et al.* [308]	2020	ANN	Inverse design
80	Akashi, Toma, and Kajikawa [152]	2020	ANN	Inverse design
81	Phan, Nguyen, Linh, *et al.* [153]	2020	ANN	Inverse design
82	Tao, You, Zhang, *et al.* [145]	2020	ANN	Surrogate model
83	Chen, Lu, Karniadakis, *et al.* [154]	2020	physics-informed neural networks (PINNs)	Inverse design
84	Harper, Coyle, Vernon, *et al.* [110]	2020	Pseudo autoencoder	Inverse design
85	Liu, Raju, Zhu, *et al.* [309]	2020	VAE	Inverse design
86	Sağık, Karaaslan, Ünal, *et al.* [311]	2021	ANN	Inverse design
87	Ma, Liu, Kudyshev, *et al.* [312]	2021	Deep Learning	Inverse design
88	Zheng, Zhang, Chen, *et al.* [311]	2022	ANN	Optimization framework
89	Trinh, Guilleminot, Perrot, *et al.* [290]	2022	Transfer Learning	Inverse design
90	Zhang, Qian, Fan, *et al.* [313]	2022	Transfer Learning	Inverse design
91	Fan, Qian, Jia, *et al.* [314]	2022	Transfer Learning	Inverse design
92	Badloe, Lee, and Rho [315]	2022	ANN	Inverse design
93	Zhou, Qiu, Zhang, *et al.* [316]	2022	ANN	Optimization framework
94	Chen, Hu, Zhu, *et al.* [317]	2023	ANN	Inverse design
95	Liu and Yu [318]	2023	Deep Learning	Inverse design
96	Zhou, Qiu, Zhang, *et al.* [316]	2023	Deep Learning	Inverse design

End of Table 1

Table 2: Table summarizing papers that use ML (except ANN) in metamaterials design.

Publication	Year	Method(s)	Application of AI
Application field: Acoustics			

Continuation of Table 2

	Publication	Year	Method(s)	Application of AI
97	Bacigalupo, Gnecco, Lepidi, *et al.* [127]	2016	Nonlinear programming	optimization framework
98	Amirkulova and Norris [103]	2018	Gradient-descent	optimization framework
99	Ghattas, Chen, and Villa [319]	2019	Bayesian Optimization	Optimization framework
100	Luo, Li, Li, *et al.* [320]	2020	Bayesian Optimization	Fuzzy Design
101	Aybike and KİLİMCİ [321]	2021	SVM,naive Bayes, decision trees	Classification
102	Tran, Amirkulova, and Khatami [322]	2022	Bayesian Optimization, Gussian Process (GP)	optimization framework
103	Jin, Zeng, Wen, *et al.* [323]	2022	Gradient-descent	Inverse Design
104	Chen, Chen, Xu, *et al.* [324]	2022	Gradient-descent	Inverse Design
105	Chang, Wang, and Dong [325]	2022	Bayesian Optimization	Optimization framework
106	Hu, Wang, Du, *et al.* [326]	2023	Bayesian Optimization	Optimization framework
	Application field: Electromagnetics			
107	Sakurai, Yada, Simomura, *et al.* [327]	2019	Bayesian optimization	optimization framework
108	Pita Ruiz, Amad, Gabrielli, *et al.* [101]	2019	Gradient-descent and Opological -derivative-based optimization	optimization framework
109	Kurniawati, Putri, and Ningsih [123]	2020	Random forest regression	optimization framework
110	Zhang, Wang, Xu, *et al.* [328]	2022	Bayesian Optimization	Optimization framework
111	Chuma and Rasmussen [329]	2022	KNN,SVM,Bayesian Optimization	Optimization framework
112	Jian, Alexandropoulos, Basar, *et al.* [330]	2022	KNN,SVM,Bayesian Optimization	Optimization framework
113	Alharbi, Abdelhamid, Ibrahim, *et al.* [331]	2023	KNN,SVM,Gradient-based Optimization	Optimization framework
114	Lin, Zheng, Hu, *et al.* [332]	2023	Bayesian Optimization	Optimization framework
	Application field: Mechanical			
115	Morris and Seepersad [333]	2018	Spectral clustering	Classification and clustering
116	Bessa, Glowacki, and Houlder [130]	2019	Bayesian ML	Classification and clustering
117	Singleton, Cheer, and Daley [100]	2019	Gradient-descent	optimization framework
118	Dong, Chen, Zeng, *et al.* [129]	2019	Nelder-Mead optimization	optimization framework
119	Stern, Arinze, Perez, *et al.* [334]	2020	Nonlinear programming	optimization framework
120	Liu, Ye, Silva Izquierdo, *et al.* [335]	2022	SVM	classification
121	Prasanna, Shantha, Pradeep, *et al.* [336]	2022	SVM ,KNN	Optimization Framework
122	Zhai and Yeo [337]	2023	Bayesian Learning	inverse design
123	Hu, Wang, Du, *et al.* [338]	2023	Bayesian Optimization	inverse design
124	Hu, Zhan, Wang, *et al.* [339]	2023	LS-SVM	Optimization Framework
	Application field: Optics			
125	Brunton, Kutz, Fu, *et al.* [340]	2015	Sparse representation for classification	optimization framework
126	Wormser, Wein, Stingl, *et al.* [102]	2017	Gradient-descent	optimization framework
127	Mansouree and Arbabi [99]	2019	Gradient-descent	optimization framework
128	Xu, Grinberg, Melati, *et al.* [341]	2019	PCA	Classification and clustering
129	Chuma and Rasmussen [342]	2022	SVM,KNN,Naive bayes gaussian	Classification
130	Hu, Li, Chen, *et al.* [343]	2022	LS-SVM	Optimization Framework
131	Zhang, Wang, Xu, *et al.* [344]	2022	Bayesian Optimization	Optimization Framework
132	Ahmadpour, Yetisen, and Tasoglu [345]	2023	Bayesian Optimization	Optimization Framework
133	Khaleel and Mudhafer [346]	2023	Navie Bayes	Classification

End of Table 2

Table 3: Table summarzing papers that use nature-inspired AI in metamaterials design.

	Publication	Year	Method(s)	Application of AI
	Application field: Acoustics			
134	Hedayatrasa, Kersemans, Abhary, *et al.* [347]	2018	GA	Topology optimization
135	Yeh and Harne [348]	2019	GA	optimization framework
136	Meng, Chronopoulos, and Fabro [349]	2019	GA	optimization framework
137	Yuan, Chen, Tan, *et al.* [350]	2019	GA	optimization framework

Continuation of Table 3

	Publication	Year	Method(s)	Application of AI
138	Liu, Cai, and Wang [351]	2020	GA	Inverse design
139	Pomot, Payan, Remillieux, *et al.* [184]	2020	GA	optimization framework
140	Xie, Wang, and Mei [352]	2020	GA	optimization framework
141	Wu, Hu, Wang, *et al.* [247]	2020	Evolutionary Algorithm	Optimization Framework
142	Wang and Liu a82	2021	GA	Optimization Framework
143	Wang and Liu [354]	2021	GA	Optimization Framework
144	Qiu and Jin [355]	2021	GA	Optimization Framework
145	Gao *et al.* [356]	2021	GA	Inverse Design
146	Li, Luo, Zhang, *et al.* [357]	2021	GA	Topology Optimization
147	Vazquez Torre, Brunskog, Cutanda Henriquez, *et al.* [358]	2021	GA	Topology Optimization
148	Wu, Hu, Wang, *et al.* [353]	2022	GA	Parametric Optimization
149	Dos Reis and Karathanasopoulos [359]	2022	GA	Inverse Design
150	Sun, Zhang, Guo, *et al.* [360]	2022	GA	Topology Optimization
151	Panahi, Hosseinkhani, Frangi, *et al.* [361]	2022	GA	Optimization Framework
152	Long, Zhu, Gu, *et al.* [362]	2022	GA	Inverse Design
153	Jian, Tang, Hu, *et al.* [363]	2022	Adaptive GA	Optimization Framework
154	Morris, Wang, Plaisted, *et al.* [31]	2023	GA	Optimization Framework
155	Zhang, Li, Wang, *et al.* [364]	2023	GA	Optimization Framework
156	Xiong, Lee, and Qin [365]	2023	GA	Optimization Framework
157	Steklain, Adames, and Ganacim [366]	2023	GA	Optimization Framework
158	Li, Sun, Wu, *et al.* [367]	2023	GA	Inverse Design
	Application field: Electromagnetics			
159	Li, Chen, Zeng, *et al.* [368]	2017	Adaptive GA	optimization framework
160	Zhang and Cuii [369]	2017	BPSO	optimization framework
161	Ahmed, Chandra, and Al-Behadili [370]	2017	GA	Inverse design
162	Han, Cao, Gao, *et al.* [371]	2017	GA	optimization framework
163	Pfeiffer and Tomasic [372]	2017	GA	optimization framework
164	Pelluri and Appasani [373]	2017	GA	optimization framework
165	Feng, Chen, and Huang [374]	2017	GA	optimization framework
166	Allen, Dykes, Reid, *et al.* [375]	2017	GA	optimization framework
167	Ding, Zhang, Zhang, *et al.* [376]	2017	GA	optimization framework
168	Mahdi and Taha [377]	2017	GA	Topology optimization
169	Su, Lu, and Li [378]	2017	PSO	optimization framework
170	Orlandi [379]	2018	Differential evolution (DE) algorithm	optimization framework
171	Bağmancı, Karaaslan, Altıntaş, *et al.* [380]	2018	GA	optimization framework
172	Lim, Song, Kim, *et al.* [381]	2018	GA	optimization framework
173	Corrêa, Resende, Bicalho, *et al.* [382]	2018	GA	optimization framework
174	Kumar, Behera, and Suraj [383]	2018	GA	optimization framework
175	Clemens, Iskander, Yun, *et al.* [189]	2018	Hybrid genetic programming	optimization framework
176	Soltani, Soltani, and Aguili [384]	2019	GA	Inverse design
177	Ibili, Karaosmanoglu, and Ergul [385]	2019	GA	optimization framework
178	Seshadri and Gupta [386]	2019	GA	optimization framework
179	Nanda, De, Sahu, *et al.* [387]	2019	GA	optimization framework
180	Assal, Benzerga, Sharaiha, *et al.* [388]	2019	GA	optimization framework
181	Karatzidis, Kantartzis, Pyrialakos, *et al.* [389]	2019	GA	optimization framework
182	Tian and Li [390]	2019	GA	optimization framework
183	Yuan, Ma, Sui, *et al.* [391]	2019	GA	Topology optimization
184	Yanzhang and Jinghao [392]	2019	GA	Topology optimization
185	Sui, Ma, Chang, *et al.* [393]	2019	IAGA	optimization framework
186	Steckiewicz and Choroszucho [394]	2019	PSO	optimization framework
187	Hao, Du, and Zhang [395]	2019	PSO-FSP	optimization framework
188	Gupta, Saxena, and Bhatia [396]	2020	BFPSO	optimization framework
189	Xie, Li, and Dong [397]	2020	GA	Inverse design
190	Abdulkarim, Deng, Luo, *et al.* [398]	2020	GA	optimization framework
191	Hameed, Shawkat, and Al-Badri [399]	2020	GA	optimization framework
192	Borzooei, Rezagholizadeh, and Biabanifard [400]	2020	GA	optimization framework
193	Abdulkarim, Deng, Karaaslan, *et al.* [401]	2020	GA	optimization framework
194	Duan, Zhang, Wang, *et al.* [179]	2020	GA	optimization framework
195	Allen, Dykes, Reid, *et al.* [402]	2020	GA	optimization framework

	Publication	Year	Method(s)	Application of AI
		Continuation of Table 3		
196	Zhu, Wang, Sun, *et al.* [403]	2020	GA	optimization framework
197	Zhu, Wang, Sui, *et al.* [404]	2020	GA	optimization framework
198	Tung, Ha-Van, and Seo [405]	2020	GA	optimization framework
199	Suraj, Behera, and Badhai [406]	2020	GA	optimization framework
200	Jiang, Li, Li, *et al.* [407]	2020	GA	optimization framework
201	Whiting, Kang, Campbell, *et al.* [408]	2020	GA	optimization framework
202	Cui, Xu, Yu, *et al.* [409]	2020	GA	optimization framework
203	Thomes, Mosquera-Sánchez, and De Marqui [410]	2020	GA	optimization framework
204	Nguyen, Bui Bach, Bui, *et al.* [411]	2020	genetic programming (GP)	optimization framework
205	Li and Yang [412]	2020	NSCGA	optimization framework
206	Li and Yang [413]	2020	NSCGA	optimization framework
207	Yang, Huang, Song, *et al.* [414]	2020	PSO	optimization framework
208	Papathanasopoulos and Rahmat-Samii [415]	2020	PSO	optimization framework
209	Diaz, Burckel, Adomanis, *et al.* [416]	2021	GA	optimization framework
210	Ahmadi, Vaezi, Harzand, *et al.* [417]	2021	GA	optimization framework
211	Gonçalves, Mesquita, and Silva [418]	2021	GA	optimization framework
212	Mayer, Bi, Griesse-Nascimento, *et al.* [419]	2022	GA	Optimization framework
213	Zong, Zhu, Yu, *et al.* [420]	2022	GA	Inverse Design
214	Liu, Wang, Olivier, *et al.* [421]	2022	GA	Inverse Design
215	Luo, Lan, Nong, *et al.* [422]	2022	GA	Inverse Design
216	Nguyen and Seo [423]	2022	GA	Inverse Design
217	Lu, Gao, and Dai [424]	2022	GA	Inverse Design
218	Sun, Jiang, and Wang [425]	2023	GA	Optimization Framework
219	Feng, Zhang, Cheng, *et al.* [426]	2023	GA	Optimization Framework
220	Zhang, Duan, Liu, *et al.* [427]	2023	GA	Optimization Framework
	Application field: Mechanical			
221	Kim, Yang, Hwang, *et al.* [428]	2017	GA	optimization framework
222	Abdeljaber, Avci, Kiranyaz, *et al.* [429]	2017	GA	optimization framework
223	Palermo, Vitali, and Marzani [190]	2018	Augmented Lagrangian Genetic Algorithm (ALGA)	optimization framework
224	Callanan, Ogunbodede, Dhameliya, *et al.* [430]	2018	GA	Inverse design
225	Bakır, Dalgaç, Ünal, *et al.* [431]	2019	GA	optimization framework
226	Wang, Sun, Li, *et al.* [432]	2019	GA	optimization framework
227	Meng, Chronopoulos, Fabro, *et al.* [433]	2020	GA	optimization framework
228	Chen, Moughames, Ji, *et al.* [434]	2020	GA	optimization framework
229	Qiu, Wang, Xie, *et al.* [435]	2020	GA	optimization framework
230	Ghachi, Alnahhal, Abdeljaber, *et al.* [436]	2020	GA	optimization framework
231	Królikowski, Blazejewski, and Knitter [437]	2020	GA	optimization framework
232	Yang, Yang, and Lo [438]	2020	GA	optimization framework
233	Bacigalupo, Gnecco, Lepidi, *et al.* [439]	2021	Adaptive optimization algorithm	Surrogate model
234	Wang, Callanan, Ogunbodede, *et al.* [440]	2021	GA	Inverse design
235	Hashemi, McCrary, Kraus, *et al.* [87]	2021	GA	optimization framework
236	Li, Luo, Zhang, *et al.* [441]	2021	GA	Topology optimization
237	Wang and Liu [84]	2021	multi island GA	optimization framework
238	Chen, Yan, Feng, *et al.* [442]	2021	PSO	optimization framework
239	Wang, Zeng, Wang, *et al.* [443]	2022	GA	Inverse Design
240	Dos Reis and Karathanasopoulos [444]	2022	GA	Inverse Design
241	Dong, Hu, Holmes, *et al.* [445]	2022	GA	Optimization Framework
242	Dong and Wang [248]	2022	GA	Optimization Framework
243	Panahi, Hosseinkhani, Frangi, *et al.* [446]	2022	GA	Optimization Framework
244	Liu and Acar [447]	2023	GA	Optimization Framework
245	Zeng, Duan, Zhao, *et al.* [448]	2023	GA	inverse Design
246	Cerniauskas and Alam [10]	2023	GA	Optimization Framework
247	Cerniauskas and Alam [182]	2023	GA	Optimization Framework
248	Cerniauskas and Alam [183]	2023	GA	Optimization Framework
	Application field: Optics			
249	Sugino, Ishikawa, Hayashi, *et al.* [449]	2017	GA	optimization framework

Continuation of Table 3

	Publication	Year	Method(s)	Application of AI
250	Sun, Cai, and Wang [450]	2017	PSO	optimization framework
251	Huang, Pu, Zhao, *et al.* [451]	2018	GA	optimization framework
252	Karaaslan, Bağmancı, Ünal, *et al.* [452]	2018	GA	optimization framework
253	Bor, Babayigit, Kurt, *et al.* [453]	2018	GA	optimization framework
254	Mayer and Lobet [454]	2018	GA	optimization framework
255	Dubajić, Daničić, Vuković, *et al.* [455]	2018	GA	optimization framework
256	Franco Rêgo, Gomes De Souza, and Rodriguez-Esquerr [456]	2018	GA	optimization framework
257	Thompson and Pisano [188]	2018	micro Genetic Algorithm	Inverse design
258	Ren, Liu, Dong, *et al.* [457]	2018	PSO	optimization framework
259	Parvez, Rao, and Zanjani [458]	2019	GA	Inverse design
260	Blechman, Almeida, Sain, *et al.* [459]	2019	GA	optimization framework
261	Zanjani, Chaharmahali, Biabanifard, *et al.* [460]	2019	GA	optimization framework
262	Mayer and Lobet [461]	2019	GA	optimization framework
263	Ma and Zhang [462]	2019	GA	optimization framework
264	Yeh and Harne [463]	2019	GA	optimization framework
265	Li, Stan, Czaplewski, *et al.* [187]	2019	micro Genetic Algorithm	optimization framework
266	Li, Bao, Jiang, *et al.* [464]	2019	PSO	Inverse design
267	Chaharmahali, Soltani, Hoseini, *et al.* [465]	2020	GA	Inverse design
	Shuai, Zhang, Xu, *et al.* [466]	2020	GA	Inverse design
268	Jiang and Yi [467]	2020	GA	Inverse design
269	Lari, Vafapour, and Ghahraloud [468]	2020	GA	optimization framework
270	Cai, Sun, Wang, *et al.* [469]	2020	GA	optimization framework
271	Liu, Maier, and Li [470]	2020	GA	optimization framework
272	Melo, Ribeiro, Benevides, *et al.* [471]	2020	GA	optimization framework
273	Li, Liu, Long, *et al.* [472]	2020	GA	optimization framework
274	DIaz, Burckel, Adomanis, *et al.* [473]	2020	GA	optimization framework
275	Mayer, Griesse-Nascimento, Bi, *et al.* [474]	2020	GA	optimization framework
276	Briones, Carrillo, and Ruiz-Cruz [475]	2020	PSO	optimization framework
277	Vafapour, Ghahraloud, Keshavarz, *et al.* [476]	2021	GA	optimization framework
278	Jin, Yang, Xu, *et al.* [477]	2021	PSO	optimization framework
279	Dadkhahfard [478]	2021	PSO	optimization framework
280	Hong, Son, Kim, *et al.* [479]	2021	PSO	optimization framework
281	Luo, Lan, Nong, *et al.* [480]	2022	GA	Inverse Design
282	Dong, Hu, Holmes, *et al.* [481]	2022	GA	optimization framework
283	Mayer, Bi, Griesse-Nascimento, *et al.* [482]	2022	GA	optimization framework
284	Sahraeian and Emami [483]	2022	GA	optimization framework
285	Zhang, Zhang, Zhang, *et al.* [484]	2022	GA	Inverse Design
286	Zong, Zhu, Yu, *et al.* [485]	2023	GA	optimization framework
287	Morris, Wang, Plaisted, *et al.* [486]	2023	GA	optimization framework
288	Morris, Wang, Plaisted, *et al.* [487]	2023	GA	optimization framework

End of Table 3

Table 4: Table summarizing papers that use multiple AI techniques in metamaterials design.

	Publication	Year	Method(s)	Application of AI
	Application field: Acoustics			
289	Bacigalupo, Gnecco, Lepidi, *et al.* [131]	2019	ANN and Quasi-Monte Carlo sequences	optimization framework
290	Wu, Liu, Jahanshahi, *et al.* [5]	2021	ANN and Reinforced learning algorithm	Surrogate model
291	Wu, Liu, Jahanshahi, *et al.* [488]	2021	ANN	surrogate Model
292	Garland, White, Jensen, *et al.* [489]	2021	CNN, Genetic Algorithm	Optimization framework
293	Jin, He, Wen, *et al.* [490]	2022	ANN	Inverse Design
294	Kennedy, Lim, *et al.* [237]	2022	Deep Learning	Optimization Framework
295	Li, Guo, Sun, *et al.* [491]	2022	Genetic Algorithm	Topology Optimization
296	Liu, Xie, Huang, *et al.* [492]	2022	Deep Learning	3D-Printing

Continuation of Table 4

	Publication	Year	Method(s)	Application of AI
297	**130 130**	2023	Gradient-based Method	Optimization Framework
298	Wang, Chen, Xu, *et al.* [493]	2023	ANN	Inverse Design
	Application field: Electromagnetics			
299	Pandeeswari, Raghavan, Krishnan, *et al.* [106]	2012	ANN and Scaled conjugate gradient	Surrogate model
300	Luna, Vasconcelos, and Cruz [86]	2013	GA and ANN	optimization framework
301	Orlandi [494]	2018	GA and ANN	optimization framework
302	Zhang, Liu, Wan, *et al.* [199]	2019	CNN and binary PSO	Surrogate model
303	Boddeti, Alabassi, Aggarwal, *et al.* [112]	2019	GA and Gradient-descent	optimization framework
304	Mercy Kingsta and Seyatha [495]	2019	GA, pattern search	optimization framework
305	Song, Zhao, and Tang [201]	2019	PSO and ANN	optimization framework
306	Harper and Mills [175]	2020	ANN and Bayesian optimization	optimization framework
307	Zhu, Qiu, Wang, *et al.* [186]	2020	GA and ANN	Inverse design
308	Prabhakar, Babu, Adinarayana, *et al.* [496]	2020	GHGWO, PSO, BFO	optimization framework
309	Bakale, Nandgaonkar, and Deosarkar [497]	2020	PSO, GA	optimization framework
310	Calik, Belen, Mahouti, *et al.* [174]	2021	ANN and Bayesian optimization	optimization framework
311	Yu and Liu [498]	2021	GA with load-resistors matrix decomposition	optimization framework
312	Hamdan [499]	2023	K-Mean clustering	Inverse Design
313	Hamdan [500]	2023	K-Mean clustering, ANN	Design Space Reduction
314	Mahouti, Belen, Tari, *et al.* [501]	2023	Bayesian Optimization, ANN	Inverse Design
	Application field: Mechanical			
315	Chen, Skouras, Zhu, *et al.* [122]	2018	Gaussian mixture model	Classification and clustering
316	White, Arrighi, Kudo, *et al.* [97]	2019	ANN and Gradient-based nonlinear programming	Topology optimization
317	Bostanabad, Chan, Wang, *et al.* [117]	2019	Globally approximate Gaussian process	Inverse design
318	Bostanabad, Chan, Wang, *et al.* [118]	2019	Globally approximate Gaussian process	Inverse design
319	Singleton, Cheer, and Daley [502]	2019	PSO, GA, HGA	optimization framework
320	Chen and Gu [95]	2020	ANN and Gradient-descent	Inverse design
321	Wu, Liu, Wang, *et al.* [185]	2020	GA and CNN	optimization framework
322	Glodež, Klemenc, Zupanič, *et al.* [503]	2020	GA, DASA	Inverse design
323	Wang, Chan, Liu, *et al.* [116]	2020	k-means and ShapeDNA	Inverse design
324	Dong, Qin, and Xiao [128]	2020	Nelder-Mead, GA and ANN	Surrogate model
325	Bonfanti, Guerra, Font-Clos, *et al.* [132]	2020	Reinforced annealing, Monte Carlo and CNN	optimization framework
326	Wang, Chan, Ahmed, *et al.* [111]	2020	VAE, k-means and PCA	Inverse design
327	Garland, White, Jensen, *et al.* [40]	2021	GA and ANN	optimization framework
328	Ji, Chen, Liang, *et al.* [504]	2021	Optimal Latin hypercube technique and GA	optimization framework
329	McMillan, Öztürk, and Acar [505]	2022	PCA	Inverse Design
330	Indurkar, Karlapati, Shaikeea, *et al.* [506]	2022	GNN	Optimization Framework
331	Zhao, Zhang, Zhang, *et al.* [30]	2022	Genetic Programming	Optimization Framework
332	Mustapha, Alhiyafi, Shafi, *et al.* [507]	2023	SVM,ANN	Inverse Design
333	Zhang, Qin, Shen, *et al.* [508]	2023	Conditional GAN	Optimization Framework
	Application field: Optics			
334	Comin and Hartschuh [29]	2018	GA and ANN	optimization framework
335	Backer [98]	2019	ANN and Steepest-descent	Inverse design
336	Liu, Zhang, Dan, *et al.* [124]	2019	ANN, DecisionTree, ExtraTree, KNN and Random forest	Inverse design
337	Mukherjee, Bhattacharjee, Halder, *et al.* [126]	2019	ANN, Weighted KNN, Complex tree, Linear SVM	Classification and clustering

Continuation of Table 4

	Publication	Year	Method(s)	Application of AI
338 339	Kiarashinejad, Abdollahramezani, Zandehshahvar, *et al.* [120]	2019	Pseudo autoencoder, autoencoder and PCA	Classification and clustering
340	Liu, Zhu, Lee, *et al.* [3]	2020	ANN and Cooperative convolution algorithm	Inverse design
341	Moon, Choi, Lee, *et al.* [121]	2020	ANN, t-Stochastic Neighbor Embedding AND k-means	Classification and clustering
342	Tao, Zhang, You, *et al.* [176]	2020	GA and ANN	Surrogate model
343	Liu, Zhang, Dai, *et al.* [509]	2020	GA, PSO, multi-traversal direct-binary search and simulated annealing	optimization framework
344	Du, You, Zhang, *et al.* [125]	2021	ANN and Forest regression and Support vector regression	Surrogate model
345	Li, Chen, Xiong, *et al.* [28]	2022	MLP,CNN,RNN	Optimization Framework
346	Li, Deng, Liu, *et al.* [510]	2022	Autoencoder, GAN	Optimization Framework
347	Al-Ashwal, Al Soufy, Hamza, *et al.* [511]	2023	DNN,CNN,GAN	Optimization Framework

End of Table 4

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