Current Opinion in Solid State and Materials Science 35 (2025) 101218

Contents lists available at ScienceDirect

Current Opinion in Solid State & Materials Science

journal homepage: www.elsevier.com/locate/cossms

Machine learning for inverse design of acoustic and elastic metamaterials

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ARTICLE INFO

Keywords:
Acoustic metamaterials
Elastic metamaterials
Inverse design
Machine learning
Deep learning

ABSTRACT

Recent rapid developments in machine learning (ML) models have revolutionized the generation of images and texts. Simultaneously, generative models are beginning to permeate other fields, where they are being applied to the effective design of various structures. In the field of metamaterials, in particular, machine learning has enabled the creation of sophisticated architectures with unconventional behavior and unique properties. In this article, we review recent advancements in the ML-driven design of a particular class of artificial materials — phononic metamaterials — that are capable of programming the propagation of acoustic and elastic waves. This review includes an in-depth discussion of the challenges and future prospects, aiming to inspire the phononic community to advance this research field collectively. We hope this article will help readers understand the recent developments in generative design and build a solid foundation for addressing specific research problems that could benefit from the application of machine learning models.

1. Introduction

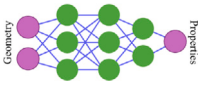
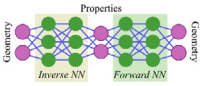
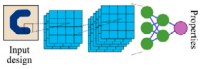
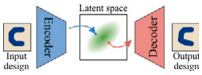
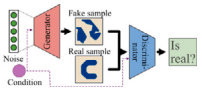
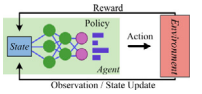
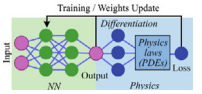
Because of the structure-dependent peculiar wave dispersion and usual properties (usually not found in nature), phononics crystals (PnCs) and phononic metamaterials (PMs) have shown tremendous opportunities for manipulating acoustic and elastic wave propagation [1]. Such an enormous phenomena occurs in frequency band gaps where wave propagation is limited. Propagation wave frequency falling inside this frequency band gap cannot propagate via periodic or aperiodic artificial structures. Therefore, it enables a potential platform for wave manipulation like wave guiding [2], focusing [3], collimation [4], wave attenuation and absorption [5]. Today, the idea of phononic crystals and metamaterials is not just restricted to theory and physical phenomena. The promising applications for noise reduction and sound proofing [6–11], aeroacoustic [12,13], automobile [14,15], underwater applications [16–18], bio-medical [19], seismic protection [20,21], and energy harvesting [22–24] are explored.

Whether discussing the unit cell or the periodic array of phononic metamaterials, optimization of structural design parameters is very important for defining the effective medium properties, and dynamic and quasi-static properties. The whole design process of such systems is usually described in two ways: (1) Forward calculations: given the structural parameters, what is the system's response? (2) Inverse calculations: given the target response, how to conceive and design the suitable structure and geometry? Brute force forward calculations are straightforward and till now many outstanding designs have been achieved using these approaches. Initial designs are tested using theoretical models or FEM-based numerical simulations [7,25–38]. To achieve the optimal response, parametric sweep is used in which design parameters are systematically varied within specified ranges. While this classical approach has shown a lot of efficiency and success, it is computationally and timely expensive for complex designs. One can only explore a tiny fraction of the solution space. Also, the whole process is guided by previous experience in phononic designs and intuitive reasoning, e.g., a cavity and a narrow neck as a building block for metamaterial absorbers due to their ability to provide quarter wavelength resonance. Despite their simple configurations and practical advantages, conventional designs face limitations in both design flexibility and achievable performance. As demand grows and functionality expands, these traditional approaches struggle to address new challenges in phononic metamaterial design, particularly when it comes to meeting the requirements of large-scale applications and user-specific features. To overcome this limit of manual and empirical design, we require fully automated design processes for on-demand realization

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https://doi.org/10.1016/j.cossms.2025.101218
Received 22 October 2024; Received in revised form 12 February 2025; Accepted 17 February 2025
Available online 5 March 2025
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Table 1
Overview of machine learning methodologies.

ML model	General architecture	General description	Common application
Multilayer Perceptron (MLP)		MLP consists of multiple layers of neurons that can learn complex input–output relationships due to non-linear activation functions applied between layers.	Function approximation, classification, regression, and inverse design of metamaterial properties (like bandgaps or waveguides) [39–41] are enhanced using MLPs with ReLU activation and dropout [42].
Tandem Neural Network (TNN)		TNN consists of two interconnected networks: one for forward mapping (design to properties) and another for inverse mapping (properties to design). Typically, the forward and inverse parts are trained separately.	Designing phononic crystals with specific bandgap widths or metamaterials for target frequencies or refractive indices [43–46].
Convolutional Neural Network (CNN)		CNN operates on pixel-based 2D and 3D structures by processing data through a series of convolutional layers. They are primarily used for image recognition, classification, and segmentation.	Image-based metamaterial designs, holograms, and acoustic absorbers [47–50].
Autoencoder (AE)/Variational Autoencoder (VAE)		AE learns efficient data representations by encoding and then reconstructing the input. VAEs extend this by incorporating probabilistic modeling, which imposes a structured lower-dimensional latent space.	Exploring material design spaces or generating new metamaterial designs with specific properties, such as bandgap size or refractive index range [51–53].
Generative Adversarial Network (GAN) (Unconditional & Conditional)		GAN consists of a generator that creates data and a discriminator that evaluates it. Conditional GANs extend this by incorporating additional labels to enable property-aware generation.	Designing dynamic metamaterials with tunable acoustic and elastic properties [54–56]. Modifications include DCGANs for high-resolution designs, Pix2Pix [57] and CycleGAN [58] for guided generation.
Reinforcement Learning (RL)		RL agents learn strategies by interacting with an environment and optimizing rewards. These agents improve their performance over time through trial and error, guided by reward signals	Adaptive optimization of dynamic metamaterials for real-time applications, such as sound insulation. [44,59,60].
Physics-Informed Neural Network (PINN)		PINN embeds physical laws, often represented as differential equations, into their loss function to enforce consistency with governing physics.	Inverse design with physics constraints [61], often using custom PINNs tailored to specific problems to search for optimal solutions [62].

of extreme physical properties or functionalities using non-intuitive designs.

In contrast to forward design, inverse design allows direct retrieval of structural parameters for the given target response (e.g., dispersion curves/bandgaps, absorption spectra, etc.) and constraints [63–67]. It is mainly focused on finding the best structure that explicitly meets the expectations. Before the recent development of machine learning techniques, inverse phononic designs frequently relied on intuitive judgments and methodical fine-tuning. A more accurate way is to use the numerical simulation methods with gradient-based (level set approach or adjoint method) [68–75] or evolutionary (simulated annealing, genetic algorithms, particle swarm optimization) algorithms [63,67,76–83]. By using this approach, the goal is to optimize design parameters to achieve a desired target functionality by minimizing (or maximizing) a fitness function. Due to the significant development of computer hardware, the ability to calculate has substantially increased and such techniques have led to remarkable success in various phononic designs by gradually refining the design problem. These algorithms use rule-based methods that involve iterative search processes tailored to individual cases. Often, they depend on numerical simulations to produce intermediate results, which help refine and adjust the search strategy. In many cases, these algorithms have proved the effectiveness for designing phononic systems and also, it does not need much human intervention. However, these stochastic methods are not sufficient for advanced design in a multi-constrained situation because of the random search character.

Machine learning, a cornerstone of artificial intelligence, enables computers to learn and improve without explicit programming. In recent years, this field has driven transformative breakthroughs across various aspects of life, including conversational AI [84,85], text-to-image generators [86], autonomous driving [87], protein structure prediction [88], medical diagnoses [89], and much more. Furthermore, there has been a notable rise in the implementation of ML techniques in the field of phononics showcase fascinating wavefront engineering features like near-perfect absorption of low frequency [49,90,91], transmission [92,93], cloaking [94], beam deflection [95], multifunctional wave control abilities [96], and many more, following their successful implementation in other areas of physics [97–101]. More specifically, integration of deep learning is proven to be greatly beneficial for high-complexity problems with large degrees of freedom [102–110]. Such data-driven approaches led to the advancement of scientific machine learning, a branch that solves the complex problems of science and engineering. In contrast to physics and rule-based approaches, ML-based algorithms automatically uncover complex relations from the given dataset. The appeal of this approach for inverse designs lies significantly in its data-driven nature and the use of feed-forward and backpropagation strategies. Machine learning has seen rapid growth through advancements in new training methods, better regularization and transfer learning techniques. Regularization in ML is a set of techniques used to ensure that a ML model can generalize to new data within the same data set [111] whereas transfer learning is a technique where a ML model trained on one task is repurposed as the foundation for other tasks. Domain-specific approaches have also improved ML's efficiency in specialized tasks. More recently, the standout development of generative models (like large language models (LLMs) and diffusion-based systems (DSs)) has significantly speed up the ability to generate new data, accelerating material discovery processes.

This article presents prominent ML models applied for the inverse design of acoustic and elastic metamaterials. Starting with the multilayer perceptron (MLP) and progressing to advanced models like physics-informed neural networks (PINNs), we present a collection of recent results that demonstrate the effectiveness of ML in the phononic

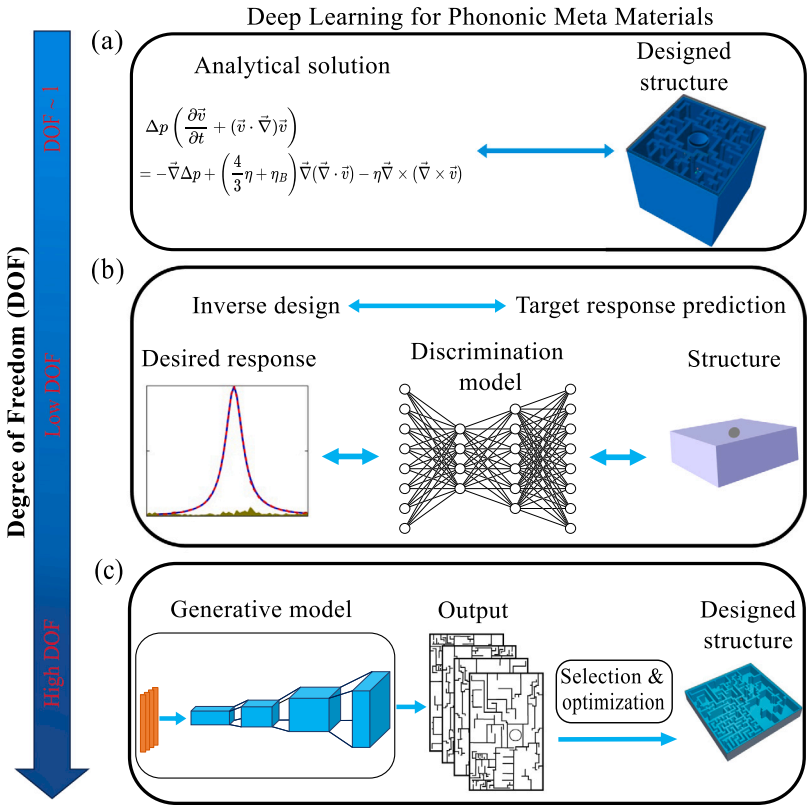


Fig. 1. Methodologies of phononic metamaterial design through deep learning at different degrees of freedoms (DOFs). (a) When the DOF of a phononic structure is low, the optimal parameter values can often be determined through analytical solutions or simple parametric sweeping. However, this straightforward design strategy may not result in the best possible performance; (b) As the DOF increases, the solution space significantly expands which necessitates exponentially increasing iterations. Discriminative models can be implemented to find relationships between design parameters and behavior of the structure. However, due to non uniqueness, a single discriminative model cannot perfectly map an output response back to a unique design parameter set; (c) When the DOF increases to thousands and more, generative networks can be employed to identify the global optimal solutions.

inverse designs where the classical design approaches are inefficient. Finally, we discuss the remaining challenges and promising potentials of this emerging multidisciplinary research field. Table 1 presents an overview of ML architectures employed in metamaterial design and analysis. The table systematically compares their architectural frameworks, practical applications, and popular use cases in the field.

2. Incorporating ML for the inverse design of acoustic and elastic metamaterials

Machine learning models used to design phononic metamaterials are highly dependent on the degrees of freedom (DOF) of the structures. Fig. 1 outlines a general framework for the implementation of ML models for various design approaches and emphasizes the role of DOFs in selecting appropriate computational methods. For structures with low DOFs, conventional methods such as parametric sweeps in analytical calculations and Finite Element Method (FEM) solvers are typically used (as illustrated in Fig. 1(a)). These approaches allow for a systematic exploration of the design space by manually adjusting a limited set of parameters, making it feasible to use brute-force simulations or calculations to identify optimal designs. As the structure becomes complex or DOFs increase, the simple parametric sweep is not sufficient to explore the whole design space due to computation power and time limitations. In order to accelerate the optimization process and to explore more design, discriminative neural networks (DNNs) are proposed as shown in Fig. 1(b). Discriminative neural networks are ML models designed for both classification and regression by learning often non-linear relationships between inputs and outputs. In classification, they establish decision boundaries to separate different categories, while in regression, they estimate continuous values based on input features. Unlike generative models, which learn the joint distribution of inputs and outputs to generate new samples, DNNs focus solely on modeling the conditional probability of an output for a given input [112]. They are particularly useful for bidirectional mapping between the design of phononic structures and their corresponding output responses. Compared to FEM simulations, trained DNNs can solve the forward problem significantly faster, often by an order of magnitude [113]. However, a key challenge arises due to the degeneracy problem, wherein multiple distinct structures may exhibit identical behavior. This makes the mapping from target responses to design structures ambiguous and necessitates additional processing to resolve these ambiguities.

When the DOFs increase to thousands, it is very difficult to optimize the whole design space which requires huge amounts of training data or too many simulation iterations. To address this, Generative Neural Networks (GNNs) are employed for dimensionality reduction. These networks simplify the representation of complex metasurface structures and their target responses, making optimization feasible by capturing the essential features with reduced parameters. Generative adversarial networks (GANs) [114] and Variational autoencoders (VAEs) [115] are the most commonly used deep generative models. GANs consist of two networks: a generator and a discriminator, which are trained simultaneously in a competitive manner. The generator generates synthetic data samples, while the discriminator evaluates whether a given sample is real or generated. This adversarial process drives the generator to produce increasingly realistic samples, effectively learning the data distribution in the original high-dimensional space. The trained GAN enables the generation of diverse designs using fewer parameters. On the other hand, VAEs use a probabilistic approach, encoding the input data into a latent space representation using an encoder network and

Table 2
ML frameworks for metamaterial design: Data, Processing, and Outputs.

ML model	Type of dataset required	Data preprocessing needs	Typical input	Typical output
Multilayer Perceptron (MLP)	Tabular datasets with structured numerical values.	Normalization, feature scaling	Numerical data (e.g., material properties, wave parameters, or geometric features)	Predicted property values or optimized material parameters
Tandem Neural Network (TNN)	Paired geometry-property datasets	Data augmentation for better generalization	Material parameters and target performance metrics	Optimized material structures that achieve target performance
Convolutional Neural Network (CNN)	Image datasets (2D/3D) or structured spatial data	Image resizing, normalization, and augmentation	Image-based data such as microstructure layouts or wave fields	Classification, segmentation, structures based on learned spatial features
Autoencoder (AE)/Variational Autoencoder (VAE)	Large-scale datasets with variations in physical properties or geometries	Dimensionality reduction and latent space regularization	High-dimensional data such as wave patterns, spectral responses, or microstructures	Compressed representations, reconstructions, or generated designs
Generative Adversarial Network (GAN) (Unconditional & Conditional)	Image-based microstructures, or paired property-structure datasets	Noise injection, conditional labeling, and adversarial loss tuning	Random noise vectors or structured conditional inputs (e.g., target bandgap size)	Synthetic designs or generated structures satisfying the given constraints
Reinforcement Learning (RL)	Simulation-based datasets dynamically generated through interactions	Reward shaping, state-space discretization, and policy optimization	State–action pairs representing material configurations in an environment	Optimizes structures obtained via learned policies for material achieving maximum cumulative reward
Physics-Informed Neural Network (PINN)	Simulated or synthetic physics-based datasets	Enforcing boundary and initial conditions, loss term balancing	Governing equations (e.g., PDEs), boundary conditions, initial conditions, and observational data	Solutions to PDEs, surrogate physics models, or physics-consistent material designs

then reconstructing it using a decoder network. The key feature of VAEs is their ability to impose a prior distribution (often Gaussian) on the latent space, ensuring smoothness and continuity. This makes it easier to sample new points in the latent space, generating new data points that are consistent with the training distribution. Once trained, GANs and VAEs can generate unlimited design variations using reduced-dimensional vectors (Fig. 1(c)). From this compact representation, an exhaustive search for the optimal structure becomes more feasible. As discussed in later sections, GNNs are often hybridized with traditional optimization algorithms to speed up the design process and overcome the issue of local minima.

3. Representative ML architectures for inverse design

Machine learning allows computational models to learn data representation at different levels of abstraction. Modern ML architectures consist of multiple (sometimes hundreds) layers of artificial neurons which perform certain transformations on the given input. By combining such transformations by all layers, the network can represent arbitrary real-valued functions. In this section, we discuss commonly used ML models based on discriminative and generative networks for inverse phononics metamaterial design. We also consider the reinforcement learning (RL) methods which involve learning optimal actions through interactions with an environment, to optimize and discover new metamaterial configurations for the desired functionalities. Finally, we discuss PINNs, which incorporates physical principles into model architecture. This integration ensures that the generated designs adhere to fundamental scientific constraints, resulting in effective device design. Table 2 summarizes the data requirements and processing steps for ML models applied to metamaterial design. It outlines the necessary input data types, preprocessing techniques, and the expected output formats for each model.

3.1. Multilayer perceptrons

A multilayer perceptron, a commonly used ML model, belongs to the class of feedforward artificial neural networks [116]. It consists of at least three layers: an input layer, one or more hidden layers, and an output layer. In each layer, artificial neurons are fully connected to those in adjacent layers through weighted connections, which is why MLPs are often referred to as "fully connected neural networks" (FCNNs). These networks use labeled data to capture complex relationships between structural parameters and the properties of AMs and EMs. The performance of an MLP is affected by its hyperparameters, which play an important role in determining the model's accuracy and generalization ability.

The inverse design problem in phononic metamaterials involves training an MLP with the target response as input and the structural parameters or design variables as output [117,118]. This approach allows the MLP to learn the mapping from desired material properties or performance metrics to the corresponding structural configurations or design parameters of the metamaterial. Liangshu et al. [117] developed an MLP-based highly accurate inverse design of topological edge states for flexural waves. The training dataset, generated using the plane wave expansion method is used to train feed-forward networks. Fig. 2(a) shows the implemented neural network architecture (the forward propagation and backpropagation cycle in black and the optimization cycle in red). Layer 1 is the input layer which sends the data to the second layer without any process. Bandgap width and 0/1 (stands for shrink/expand) are the inputs and the network is trained to generate the arrangement radius R as output. Fig. 2(b) presents the comparison of predicted value by MLP and real values (black dots). The orange line represents corresponding perfect same values. It can be observed from the plot that all black dots are perfectly on the orange line showing a highly accurate result. Fig. 2(c) represents the histogram of predicted error which is just 0.01%, making it an accurate implementation of the inverse prediction model.

While MLPs have been effectively used to solve inverse problems, they face challenges with many-to-one mappings, commonly known as the non-uniqueness issue in design problems. This limitation makes MLP less efficient for handling complex designs. To address these challenges, especially in design problems constrained by physical laws, an MLP can function as a surrogate model within an optimization algorithm. For example, as illustrated in Fig. 3, Zhou et al. [95] combined an MLP with a genetic algorithm to enable the inverse design of a multi-functional EM. This approach allows for precise manipulation of wave refraction angles, resulting in successful design outcomes.

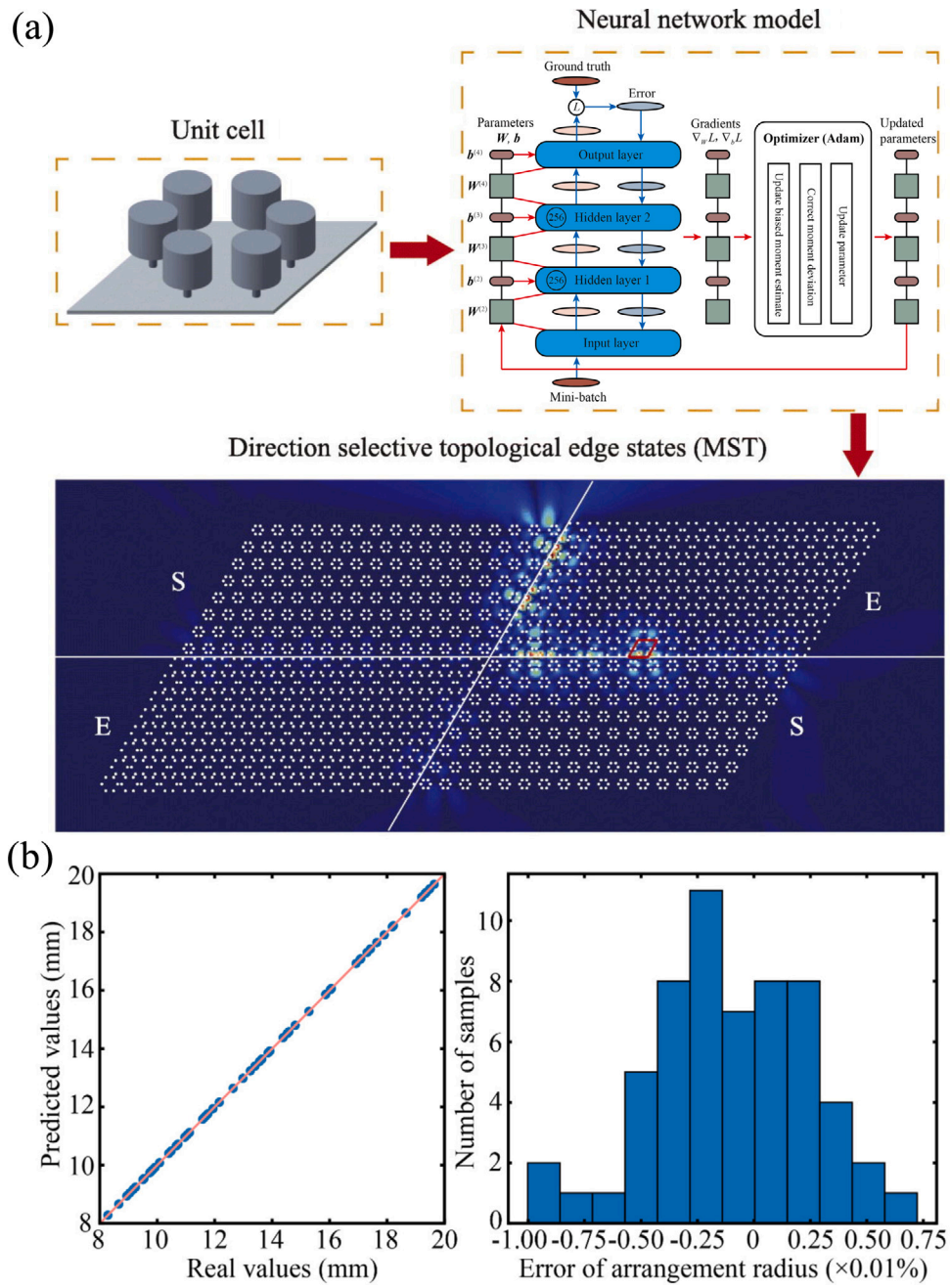


Fig. 2. MLP based inverse designs of phononic metamaterials. (a) Implemented MLP during training the forward and back propagation (black) and optimization (red). [Liangshu et al. [117], Elsevier, Reproduced with permission]; (b) Comparison of the actual value for the arrangement radius R with the predicted value. [Liangshu et al. [117], Elsevier, Reproduced with permission]; (c) Histogram of the prediction error. [Liangshu et al. [117], Elsevier, Reproduced with permission].

3.2. Tandem neural network-based model

In phononics, tandem neural networks (TNNs) are particularly suited for solving inverse problems. Such models share a structural similarity with models like AEs and GANs, as they consist of two interconnected networks: a pre-trained forward network and an inverse design network with specified input and desired output. The forward network, which operates on the principles of supervised learning, serves as a reliable prediction model. Supervised learning is a type of ML in which a model is trained on a labeled dataset, meaning each input is paired with a corresponding output. The model learns to map inputs to outputs by minimizing the error between the predicted and actual outputs during training. During training of a TNN, the weights and biases of the forward network remain fixed, while the parameters of the inverse network are optimized to minimize the cost function. In the inverse design process, the target phononic properties are input into the inverse network, and the corresponding design structures are extracted from the intermediate layer, which encodes the structural parameters. Compared to an AE, training a TNN introduces additional complexity because it requires integrating two networks and effectively coordinating their training. However, TNNs offer the benefit of directly correlating the structure with its response, eliminating the need for explicit feature extraction.

He et al. [44] implemented TNN for the inverse design and analysis of topological phononic beams, targeting applications such as robust bandgaps and localized states. This implementation helps resolve the complexity in training that arises from inconsistent data. As shown

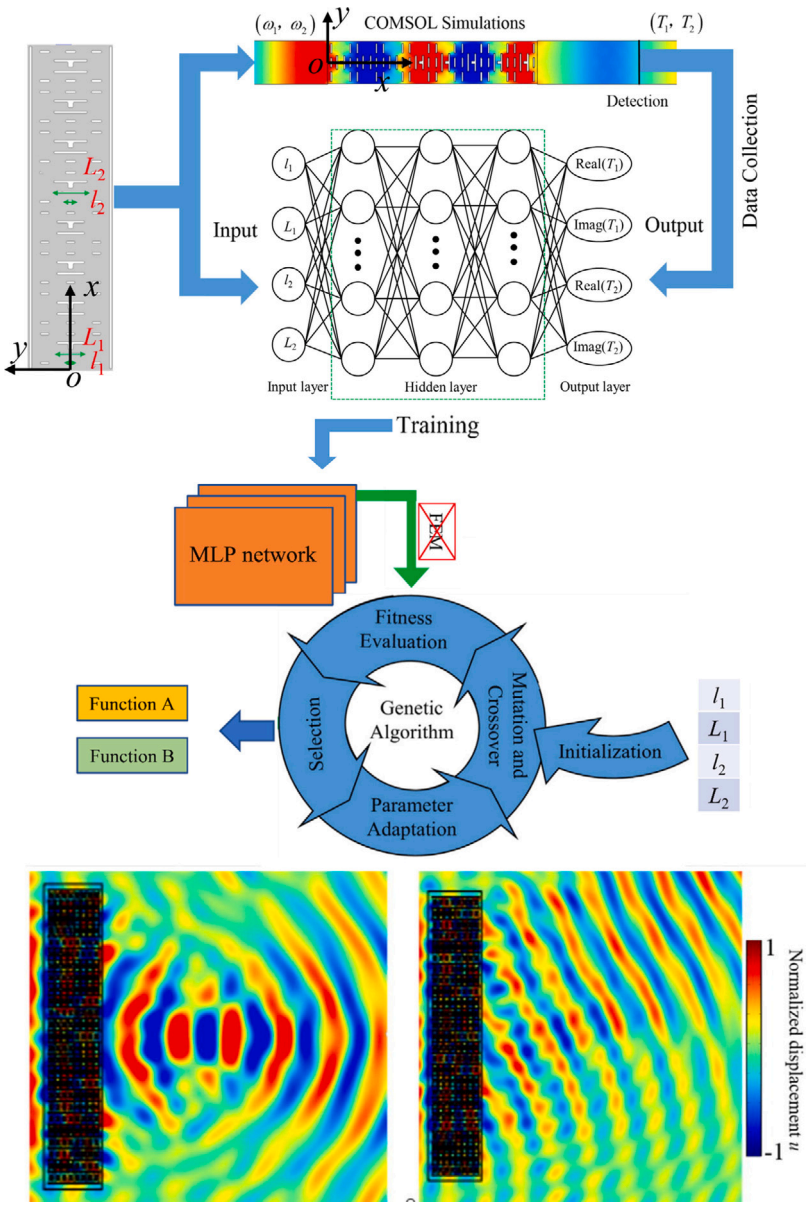


Fig. 3. Integration of MLP with Genetic algorithm for fast inverse multifunctional metasurface design. [Zhou et al. [95], Elsevier, Reproduced with permission].

in Fig. 4(a), the inverse network, I, is linked to the pre-trained forward network, F. For the forward network, a given beam structure corresponds to a single topological response, simplifying the training process. The intermediate layer generates the structure parameters based on the input's topological properties. Fig. 4(b) compares the predicted topological properties (red dots) with the actual properties (black lines) for two different cases. In a separate study, Li et al. [45] developed a TNN-based model to map the relationship between flexural wave band gaps and micro-phononic beams, as shown in Fig. 4(c). The TNN is pre-trained, and the inverse network is trained in a full loop with the assistance of the forward network. Once training is complete, designs for micro-PnC beams are generated at the output, based on the given bounding frequencies of the first and second stop bands, accounting for size effects. Fig. 4(d) presents the imaginary panels of flexural waves from random samples, comparing the generated and real samples. Li et al. [43] applied a probabilistic TNN-based approach for the inverse design of nano-sized functionally graded material PnCs having desired bandgap properties. Fig. 4(g) illustrates this model, which incorporates inverse and forward networks along with Gaussian sampling. The final comparison between predicted and actual designs, shown in Fig. 4(h), demonstrates that the predicted bounding frequencies closely match the real values. Other works have also implemented the same models for different design purposes, such as achieving super scattering underwater [119] or target sound isolation performance in laminated acoustic metamaterials [121] and optimizing the geometry of topological phononic beams [120].

When implementing TNNs for inverse design, conditional variables can be seamlessly integrated into the pre-trained forward network along with the design variables. To ensure that these conditional variables remain unchanged, it is essential to decouple them from the inverse design network. This approach provides flexibility by allowing the design of multiple distinct structures from a single target. By adjusting the hyperparameters of the TNN or modifying the initial internal parameters of the inverse design network at the outset of the design process, the system's versatility is enhanced, enabling the generation of diverse solutions for a given design objective.

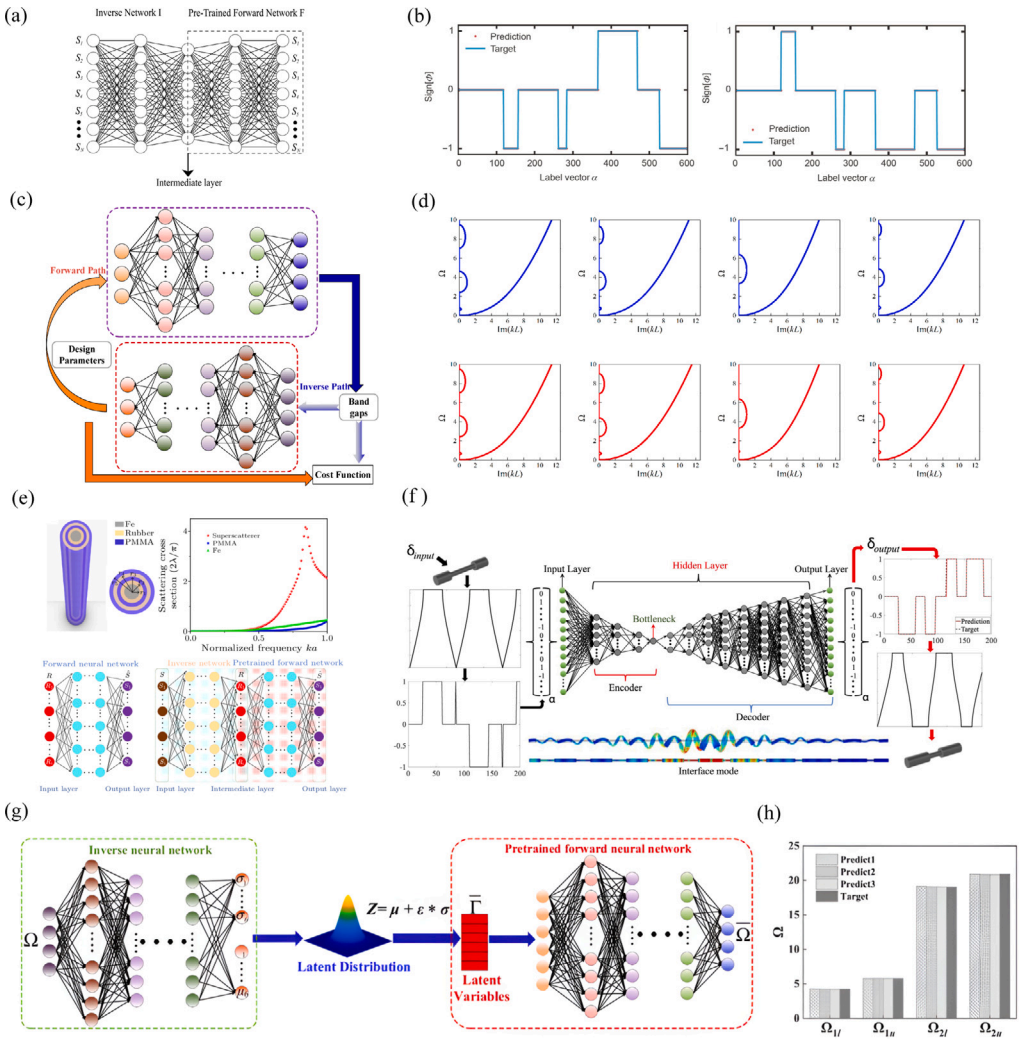


Fig. 4. TNNs for inverse design of phononic metamaterials. (a) Implemented TNN for design of phononic beam where Inverse network I is connected to pre-trained forward network F; (b) predicted and targeted topological properties. [He et al. [44], Science China Physics, Mechanics & Astronomy, Reprinted with permission. Copyright 2022, SpringerNature, under STM Permissions Guidelines]; (c) TNN employed to map the relationship between flexural wave band gaps and micro-phononic beams. [Li et al. [45], MDPI, Reproduced under the terms of the Creative Commons Attribution (CC BY) license]; (d) Imaginary panels of flexural waves corresponding to random samples (red lines and black lines represent actual and predicted values, respectively). [Li et al. [45], MDPI, Reproduced under the terms of the Creative Commons Attribution (CC BY) license]; (e) TNN to obtain super scattering of underwater sound. [Miao et al. [119], Chinese Physics Letters, Reproduced with permission]; (f) TNN for topological phononic beams. [Muhammad et al. [120], IOPscience, Reproduced under the terms of the Creative Commons Attribution (CC BY) license]; (g) Probabilistic TNN for phononic crystals design. [Li et al. [43], Elsevier, Reproduced with permission]; (h) comparison of predicted and actual values of bounding frequencies. [Li et al. [43], Elsevier, Reproduced with permission].

3.3. Convolutional neural network-based model

In phononics, MLPs and TNNs are typically implemented for the low-dimensional feature parameters. Usually, such feature parameters include geometrical and physical parameters, material properties, and boundary conditions. To deal with high-dimensional parameters, CNNs are often a better option as it is well-suited for problems involving spatial data, like images and matrices. CNNs have been effectively implemented for the forward and inverse designs in phononics due to their ability to capture complex spatial relationships [8,105,125]. Such networks primarily comprise convolutional layers, pooling layers, and fully connected layers. Convolutional layers help the model to learn spatial information by detecting local patterns. Pooling layers are used to reduce the spatial dimension of data which subsequently reduces computation cost. In CNN, fully connected layers are typically used to combine all features into a comprehensive representation of the input data.

Recently, Huang et al. [122] present a CNN-based inverse design method for 1D nonlinear phononic crystals (NPC). The input to the network is the desired transmission response and in output, it is expected from the model to predict the corresponding physical and geometrical parameters. Fig. 5(a) depicts the flowchart of the implemented design. The desired transmission response is represented by a 1×1000 1D array which is input to a trained neural network. In output, the model is expected to generate corresponding NPC material parameters (density ratio, sound velocity ratio, interface stiffness, and thickness ratio) for the given input. CNN structures with different numbers of convolutional layers and pooling layers are used for evaluating three different cases: (1) two parameters (ζ and η) (2) three parameters (ζ, η, and κ) (3) four parameters (ζ, η, κ, and λ). Fig. 5(b) shows the RMSE of the testing set with different CNNs for these all cases which shows excellent prediction accuracy. Han et al. [123] implemented a CNN-based inverse topological design of 1D periodic 2D tetragonal PnCs. Fig. 5(c) illustrates the deep learning framework where CNN and the generator of GAN are concatenated for inverse design. Here, CNN and GAN are trained one by one. Once the training is done, both networks are taken out and connected together. Fig. 5(d) demonstrates that Pix2Pix generates a nearly identical topology from the band structure, whereas Fig. 5(e) displays a different generated topology. The band

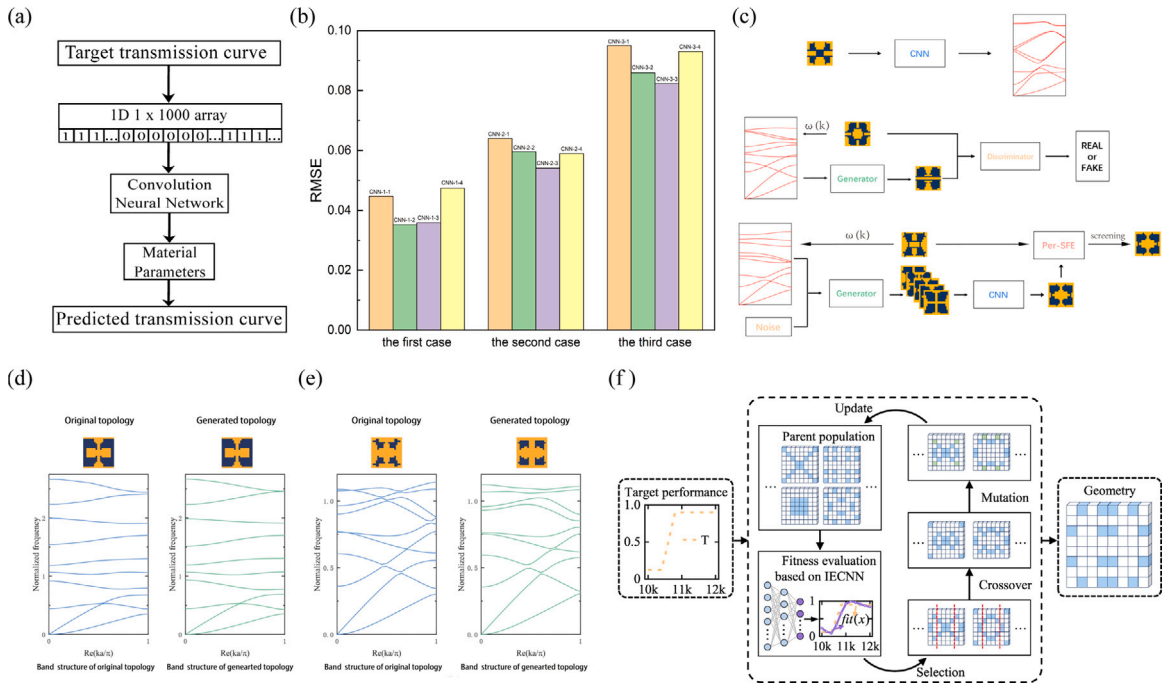


Fig. 5. Convolutional Neural Network for metamaterial design for 1D nonlinear phononics crystals. (a) Flowchart of design; (b) Root mean square values for test dataset using different CNN structures for the three cases. [Huang et al. [122], IEEE, Reproduced under the terms of the Creative Commons CC BY-NC-ND license]; (c) Implemented CNN and GAN for topology optimization. [Han et al. [123], Journal of Applied Physics, Reprinted with permission. Copyright 2022, AIP Publishing, under STM Permissions Guidelines]; (d),(e) Generated topologies and corresponding band structures. [Han et al. [123], Journal of Applied Physics, Reprinted with permission. Copyright 2022, AIP Publishing, under STM Permissions Guidelines]; (f) Integration of CNN with Genetic algorithm for inverse design of metasurface structure with specified target transmission performance. [Zhang et al. [124], Elsevier, Reproduced with permission].

characteristics of generated topologies and original topologies are similar in both cases, particularly for the lower modes. The one-to-many relationship between the topological structure and the band structure is demonstrated, opening up the possibility of inverse design and optimization. Unlike MLP, CNNs can also be used with other optimization algorithms, such as genetic algorithms for inverse designs. Recently, Zhang et al. [124] integrate Genetic Algorithm with CNN for designing metasurface structure with specified target transmission performance. Fig. 5(f) shows the implemented inverse design framework that follows a series of strategic steps to rapidly optimize the metasurface geometry for the desired performance. This approach combines the strengths of CNN for precise performance prediction in limited-sample scenarios with GA's capability for effective exploration and optimization of the design space.

3.4. Autoencoder-based model

The discriminative algorithms previously discussed are not particularly effective for addressing inverse problems characterized by high dimensionality and discrete variables, especially in cases involving non-intuitive designs. These algorithms often struggle to navigate the complex and discontinuous solution spaces typically associated with such problems, limiting their ability to generate optimal or innovative design solutions. This issue can be alleviated by converting high-dimensional data into lower-dimensional, continuous forms. Autoencoder, which consists of an encoder and a decoder, is capable of performing this kind of data compression [126]. The encoder maps input data into a lower-dimensional latent space, capturing essential features while reducing complexity. The decoder then reconstructs the data from this latent representation, functioning as a generative network where the latent space distribution serves as the input. This approach facilitates the handling of high-dimensional, discrete data by transforming it into a more manageable, continuous form, thereby improving the efficiency of solving inverse problems. Li et al. [127] implemented an AE four years ago for the topology design of a 2D PnC with anticipated band gaps, as shown in Fig. 6(a-b). A deep convolutional autoencoder can be utilized to design a hybrid sound absorber with complex geometric parameters. Fig. 6(d) presents a schematic representation of this approach, illustrating the encoder–decoder architecture used for predicting wave vector responses. More recently, Mahesh et al. [51] used a deep convolutional autoencoder to design a hybrid sound absorber, Fig. 6(e) shows comparison between predicted results with experimental outcomes which shows good agreement between both.

Despite their successful implementation, AEs face a limitation in ensuring that their latent vectors remain continuous and capable of generating new data. This constraint can restrict the design space, hindering the exploration of novel solutions or smooth interpolation between features. As a result, AEs may underperform in applications where both dimensionality reduction and creative generation are required. To address these problems, Variational Autoencoders introduce a probabilistic framework for latent vectors, offering a more regularized and smooth latent space compared to traditional AEs, thereby providing greater robustness to variations [128]. In a VAE, the encoder produces a probability distribution in the latent space, and the decoder samples from this space to reconstruct the input data. The encoder employs regularization loss, particularly KL divergence, to measure how closely the generated output matches the input. This loss function encourages the latent space to exhibit desired properties such as regularity, continuity, and organization.

Wang et al. [53] used the Gaussian mixture beta variational autoencoder (GM-β VAE) for the inverse design of phononic bandgap metamaterial. As compared to basic VAEs, GM-β VAE offers better learning ability and can generate more diversified designs. Fig. 7(a) shows the implemented design framework where VAE is integrated with MLP. The VAE transforms topologies into latent vectors and vice versa. Based on the given latent vectors, the MLP is trained to predict band gaps. Gaussian process regression models are trained to predict

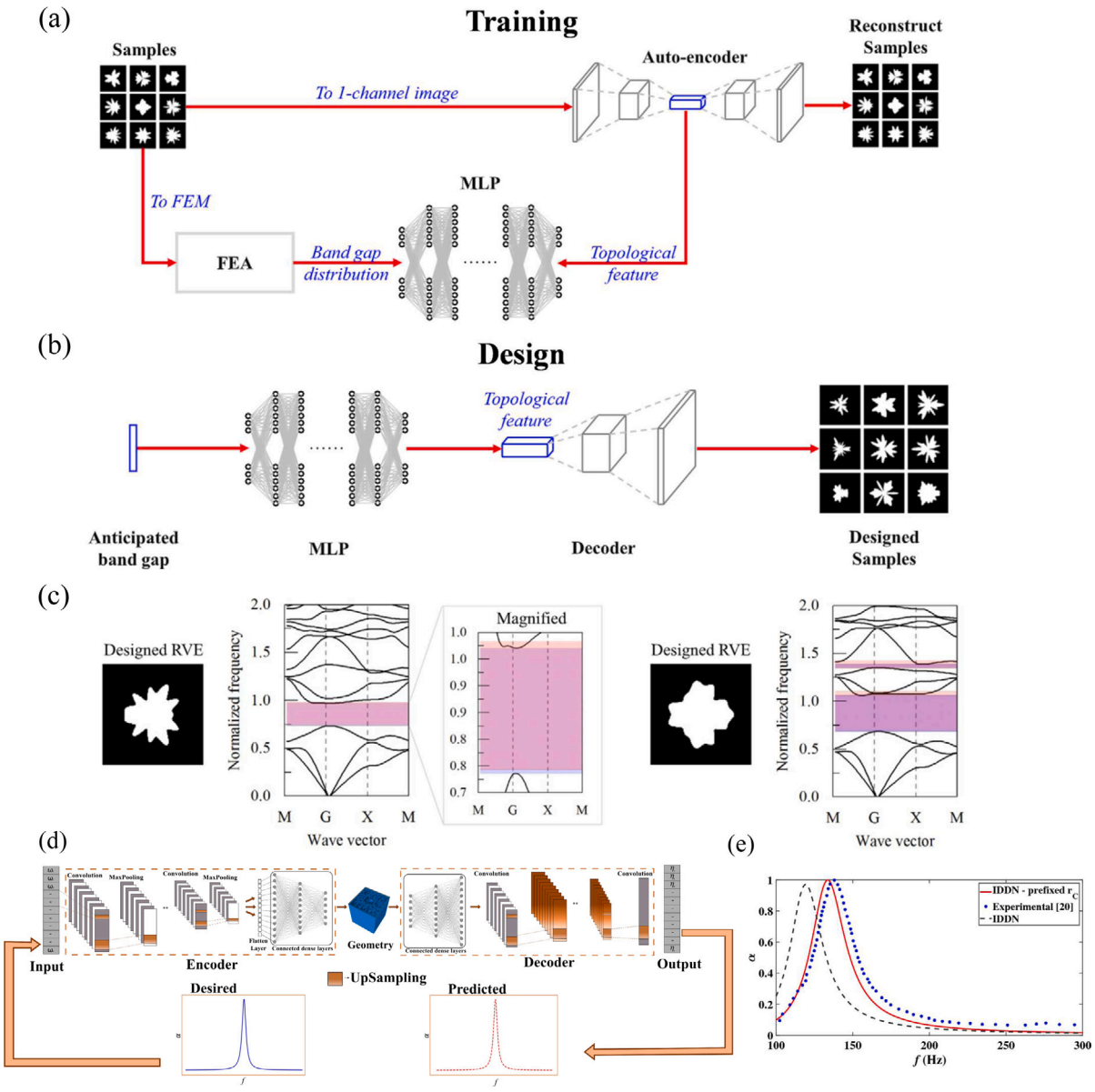


Fig. 6. AE based machine learning models for the inverse design of phononic metamaterials. (a-b) The training and design workflow for designing of PnCs with anticipated BG. [Li et al. [127], Elsevier, Reproduced with permission]; (c) Designed PnC with representative volume elements (RVEs). [Li et al. [127], Elsevier, Reproduced with permission]; (d) Implemented a deep convolutional autoencoder for the sound absorber design; (e) Comparison of predicted results with experimental results. [Mahesh et al. [51], Engineering with Computers, Reprinted with permission. Copyright 2023, SpringerNature, under STM Permissions Guidelines].

the relationship between latent features and properties for property-driven optimization. A conditional VAE (cVAE) was implemented by Dedoncker et al. [129] as shown in Fig. 7(b) for fast on-demand resonator design. For the variational encoder, the design parameters are the input and the mean and log variance of a Gaussian distribution are the output. For the encoder, the input is a point in the latent space and the requested attributes and output is the set of design parameters. The full measurement setup for the experiment is shown in Fig. 7. Encoding sound-transmission loss into the latent space of the cVAE also enables efficient designs of ventilated acoustic resonators with broadband sound attenuation [130].

3.5. Generative adversarial network-based model

A generative adversarial network is a model designed to work with high-dimensional data. Recently, such networks have been successfully implemented to identify patterns with non-intuitive topologies in the designing of AMs for desired target response [131]. Introduced in 2014, GANs consist of a pair of a generator and a discriminator [132]. A generator network produces a geometric dataset sent to the discriminator network. A discriminator also receives the patterns from the training set. A generator network produces a geometric dataset which is sent to the discriminator network that also receives the patterns from the training set. It serves as a binary classifier and decides if the pattern is coming from the training set or generator. During training, both networks compete against each other. A generator tries to fool the discriminator by generating fake patterns, which mimic the original patterns from the training set. Concurrently, a discriminator tries to differentiate real from fake patterns. Once the training is successfully over, the discriminator is unable to differentiate between real patterns from the training set and the synthetic patterns generated by the generator. During the training, the generator learns to produce patterns by capturing the underlying distribution of the training set with no explicit assumptions about its properties. As shown in Fig. 8, Zhang et al. [131] employed GAN for the topological design of metal porous

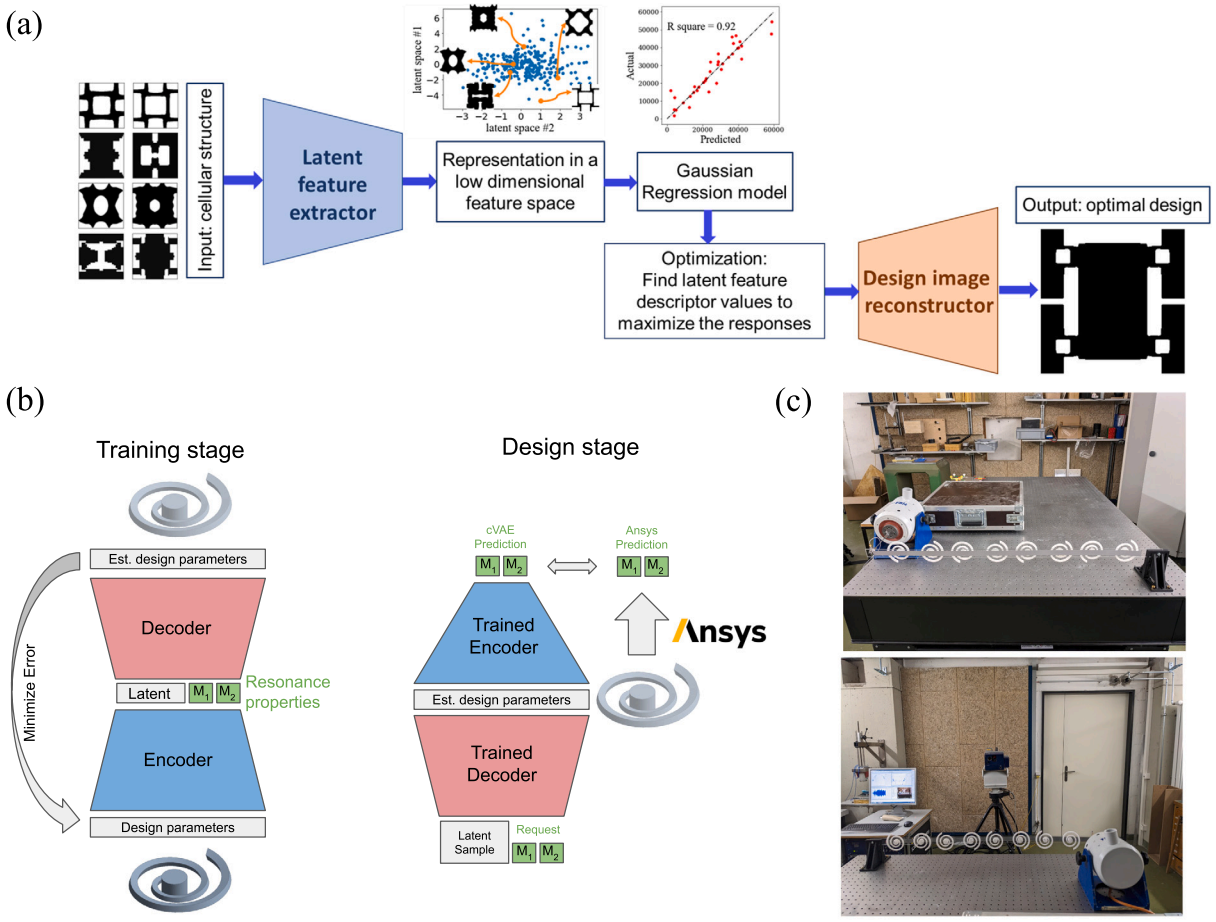


Fig. 7. Implementation of VAEs for the inverse phononic metamaterials. (a) Gaussian beta variational encoder (GB-VAE) for phononic bandgap metamaterial. [Wang et al. [53], Journal of Mechanical Design, Reprinted with permission. Copyright 2022, ASME, under STM Permissions Guidelines]; (b) Conditional VAE for resonator design. [Dedoncker et al. [129], arXiv, Reproduced under the terms of the Creative Commons CC BY-NC-ND license].;(c) Experimental setup for measuring the dispersion characteristics of the metamaterial beams. [Dedoncker et al. [129], arXiv, Reproduced under the terms of the Creative Commons CC BY-NC-ND license].

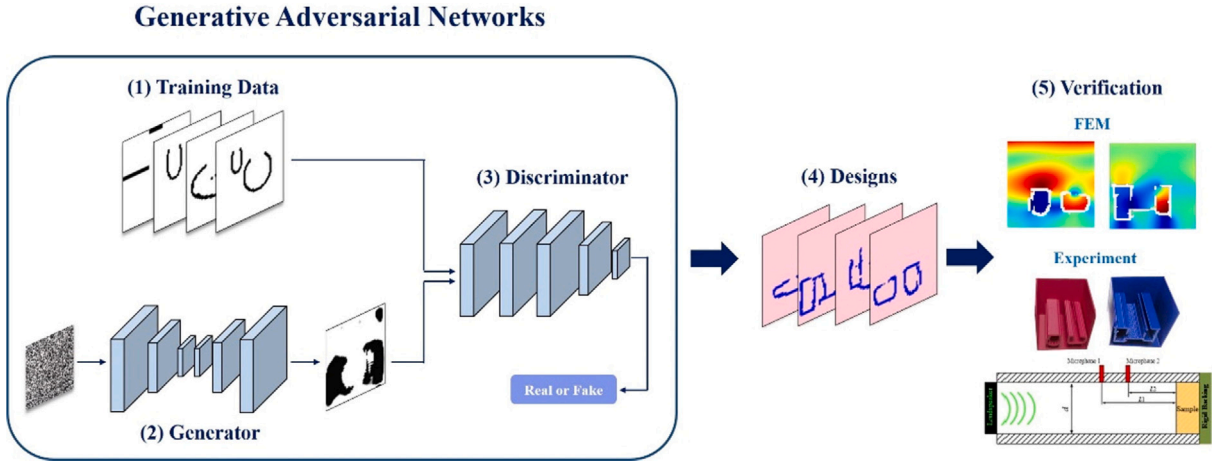


Fig. 8. Implementation of GAN for the metaporous material design for sound absorption. [Zhang et al. [131], Elsevier, Reproduced with permission].

material for sound absorption. However, for the phononics inverse designs, conditional GAN (cGAN), a variant of GAN, is more effective due to its ability to incorporate and condition additional information.

The cGAN is an extension of the traditional GAN, incorporating specific conditions derived from real sample properties in the training data. As shown in Fig. 9(a), Gurbuz et al. [133] implemented a cGAN architecture to design 2D AMs, where the generator produced cell geometries tailored for specific transmission behaviors. In another example, as shown in Fig. 9(b), Xiao et al. [54] used cGAN for the design of two-dimensional irregular elastic metamaterials (EMs), leveraging a topology dataset to efficiently generate scalable and controllable EMM designs. Jiang et al. [134] employed cGAN for the inverse design of EMs, generating dispersion curves as outputs introduced a novel approach by integrating CNNs to predict dispersion curves, refining the

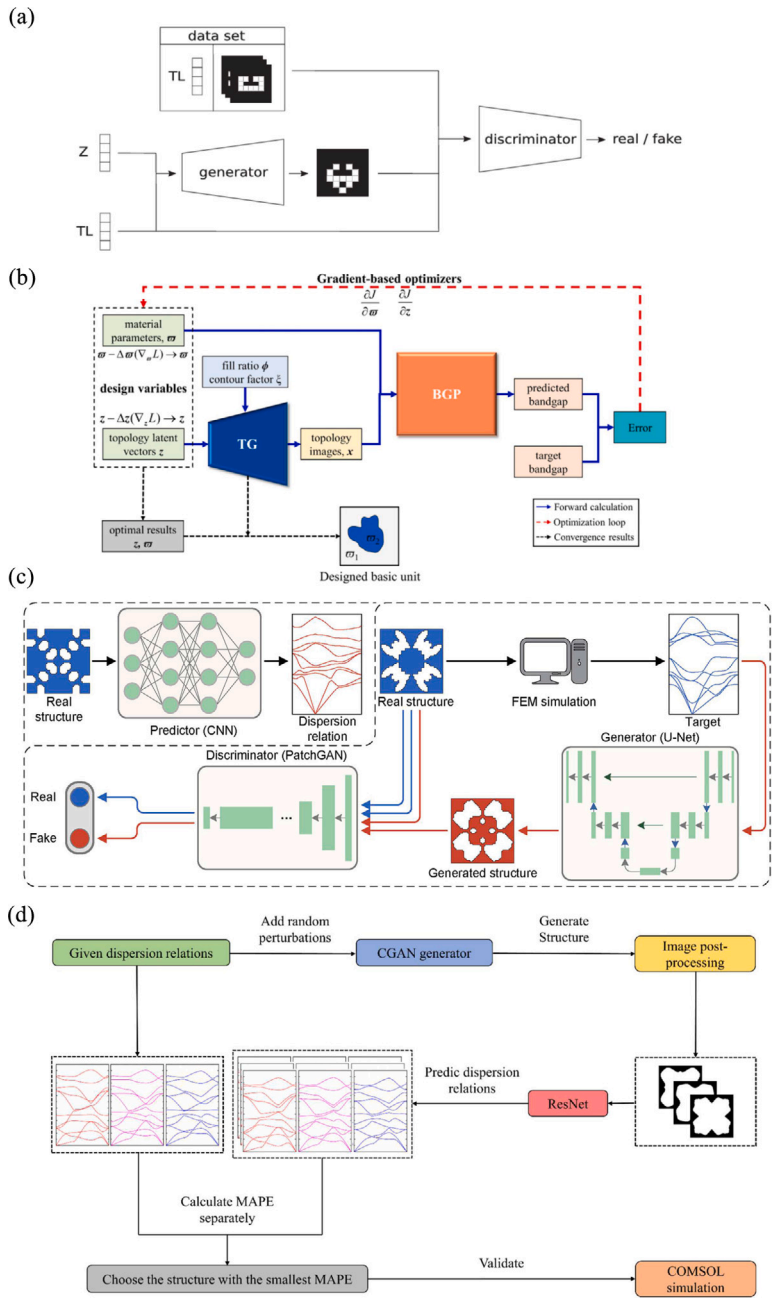


Fig. 9. Implementation of cGAN for phononic metamaterial design. (a) cGAN for 2D acoustic metamaterial design. [Gurbuz et al. [133], AIP Publishing, Reproduced under the terms of the Creative Commons CC BY license]; (b) The structural inverse design of 2D irregular elastic metamaterials. [Xiao et al. [54], Elsevier, Reproduced with permission]; (c) Integration of CNN and cGAN for dispersion curve prediction. [Jiang et al. [134], Elsevier, Reproduced with permission]; (d) Integration of ResiNet and cGAN for 2D tunable phononic crystal design [Zhou et al. [55], Elsevier, Reproduced with permission].

generator's results and enhancing accuracy (Fig. 9(c)). This method bypasses the usual probabilistic inputs of GANs, instead creating a direct link between target dispersion curves and topologies, with the discriminator ensuring output quality. Recently, Zhou et al. [55] combines cGAN with Residual Network (ResNet) to establish an inverse design framework for 2D tunable phononic crystals as shown in Fig. 9(d). ResNet helps to establish mapping from structure to dispersion relations for forward prediction which reduce the time-consuming FEM process. It is a deep learning architecture designed to train very deep networks by introducing skip connections that allow data to bypass intermediate layers, preventing vanishing gradient issues. It learns residual mappings instead of direct mappings, making optimization more efficient. In the proposed model, most samples have errors within the range of 0–1.5% which shows the effectiveness of the implemented ResNet. The whole inverse framework is based on a statistical optimization approach. Initially, dimensionality reduction is applied to the input dispersion relations, which are then augmented with random perturbations. These modified inputs are passed through the generator of a cGAN to produce multiple structural images. Afterward, these images undergo a post-processing step. The processed images are subsequently evaluated using a ResNet model to predict corresponding dispersion relations. The Mean Absolute Percentage Error (MAPE) is calculated between the provided dispersion relation and the predicted ones. The structure with the lowest MAPE is selected as the optimal design. To ensure the accuracy of the generated structures, FEM simulations are performed as a final verification step. This process combines the capabilities of cGAN and ResNet, enabling the inverse design process to bypass extensive finite element simulations, thereby improving overall efficiency.

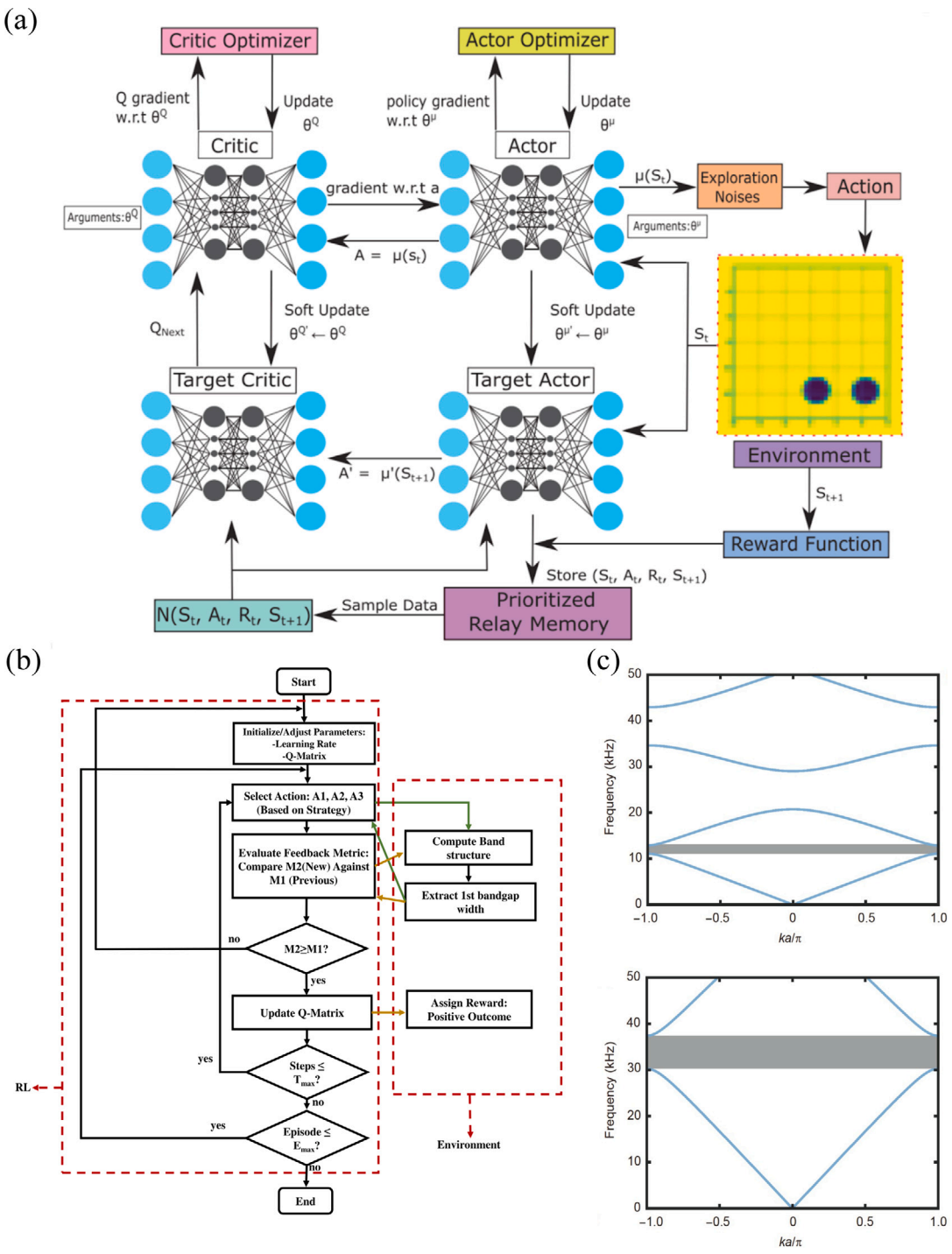


Fig. 10. Implementation of Reinforcement Learning for inverse phononic metamaterials. (a) Schematic of double deep Q-learning network (DDQN) for suppressing acoustic scattering. [Shah et al. [59], JASA, Reprinted with permission. Copyright 2021, Acoustical Society of America, under STM Permissions Guidelines]; (b) Reinforcement learning to maximize the first band gap width; (c) Dispersion diagrams of the initial and final states, respectively. [He et al. [44], Science China Physics, Mechanics & Astronomy, Reprinted with permission. Copyright 2022, SpringerNature, under STM Permissions Guidelines].

3.6. Reinforcement learning

Reinforcement Learning is a branch of ML inspired by behavioral psychology and the way environments change [60]. It reflects the human learning process by relying on trial-and-error experiences. The main goal during training is to balance exploration — trying out unfamiliar actions — and exploitation, where the focus is on using known information to maximize rewards. Unlike other ML methods, RL does not require labeled input data. The RL model has three key components: agent, environment, and reward. The agent is responsible for learning and making decisions by interacting with the environment. It selects actions, and the environment responds by updating its state. For each action, the environment provides feedback in the form of a reward. The agent aims to optimize its performance by maximizing the total reward over time through continuous interaction.

In the inverse design of PMs, geometric parameters and material properties act as agents, while the target response represents the environment. By modifying these parameters, the system's response changes, allowing the exploration of multiple design possibilities. Once trained, the model can identify the optimal structure for a specific

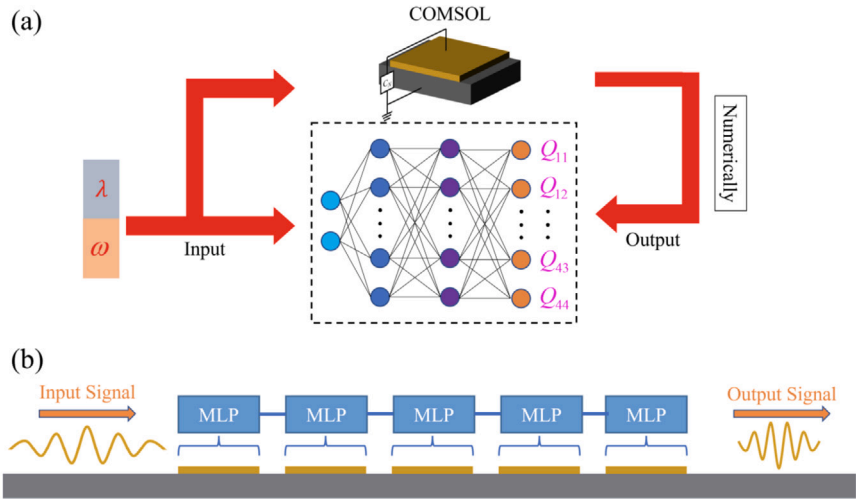


Fig. 11. Implementation of physics-informed neural networks for the prediction of the global transfer matrix. (a) illustration of the implemented ML model for a metabeam unit. [Chen et al. [96], Elsevier, Reproduced with permission]; (b) integration of ML networks for the transfer matrix calculation. [Chen et al. [96], Elsevier, Reproduced with permission].

target output. Shah et al. [59], implemented the RL algorithm, specifically a deep Q-learning approach, to suppress acoustic scattering, as shown in Fig. 10(a). The goal of the network was to determine the design parameters for acoustic cylindrical scatterers that minimize the root mean square (RMS) of the total scattering cross-section (TSCS). These parameters were optimized through an RL agent. The agent iteratively adjusted the design based on the gradients of the TSCS and relevant configuration data, while accounting for multiple scattering effects between cylinders. Each action by the agent resulted in a reward, which was inversely proportional to the RMS of the TSCS over a range of wavenumbers. Over successive episodes, the agent learned to identify configurations that effectively reduce scattering. More recently, He et al. [44] applied RL to increase the width of band gaps in a phononic beam. In their model, the dispersion relationship defined the environment, while structural parameters served as agents. The RL algorithm is trained to maximize the width of the first band gap. Fig. 10(b) shows implemented RL flowchart where the RL and environment parts are separated. The environment calculates the width of the first bandgap using an algorithm that employs a Q-function, which considers both states and actions as variables. The Q-matrix is initialized with zero values, and the Q-function updates its values based on the rewards received during each training iteration. The agent follows a ϵ-greedy strategy to select an action in the current state. Each state has six possible actions to choose from. However, if executing an action exceeds the given parameter limits, the action becomes invalid. To assign rewards and update the Q-matrix, the current bandgap width is compared with the previous state's bandgap width. Fig. 10(c) displays the initial and optimized dispersion curves. Due to the inclusion of randomness in the action selection, the parameter configuration that achieves the maximum bandgap width may not always be attained, but rather falls within a specific range of possible configurations.

3.7. Physics-informed neural network

Many of the ML algorithms discussed so far are often regarded as 'black boxes' due to their complex architectures, making it difficult to interpret or explain their inner workings. As models become more sophisticated and data-intensive, their interpretability and explainability become increasingly challenging. This issue is particularly pronounced in inverse design, where understanding how the model arrives at specific decisions is very important. Research indicates that by embedding physical laws into neural networks, models can achieve better performance with less empirical data. Additionally, incorporating prior physical knowledge enhances the model's ability to generalize beyond the training data. A PINN is an approach that integrates domain-specific physical laws into deep neural networks. This interdisciplinary method improves the analysis of physical systems by lowering data requirements, enhancing generalization, and ensuring high accuracy and faster convergence. In phononics, PINNs can incorporate fundamental physical principles, such as wave equations and boundary conditions, to predict desired responses more effectively. Recently, these models have started being applied to the forward and inverse design of PMs [135, 136].

Chen et al. [96] developed a physics-guided ML model for multi-functional wave control in an active metabeam. As shown in Fig. 11(a), an MLP is first trained to learn the underlying physics from a unit cell. After training, multiple neural networks (Fig. 11(b)) are combined to construct the global transfer matrix, enabling the prediction of the beam's dynamic response across the entire system. The model predicts and utilizes transfer matrices to capture wave propagation in the metabeam. These matrices connect the wave field with its derivatives, playing an important role in describing the beam's dynamics. By integrating the transfer matrix into the neural network, the model establishes a detailed mapping between input parameters and output wave responses. This physics-guided approach successfully achieves user-defined wave functions and facilitates the inverse design of non-periodic active metamaterials.

4. Perspectives on challenges and emerging development

This article explored various key ML algorithms for the inverse design of PMs. MLP is a basic artificial neural network architecture widely used in phononic designs. However, due to its limitations in handling complex non-linear mappings, maintaining training stability, and offering interpretability, MLPs are less effective for inverse design tasks compared to more specialized ML algorithms. TNNs leverage the property prediction capabilities of MLPs and are more effective at solving inverse design problems. CNNs, on the other hand, excel at processing image data or metrics-based datasets, making them suitable for design tasks that involve spatial or structured data. AE models transform high-dimensional, discrete problems into lower-dimensional, continuous representations. This feature makes AEs particularly valuable for tasks such as topology optimization and design refinement, where reducing complexity and capturing essential patterns is critical for efficient exploration of the design space. GANs and their variants, such as cGANs and Wasserstein GANs generate high-quality designs

Table 3
Summary of machine learning techniques in metamaterials.

ML model	Unique features	Pros	Cons	Demonstrated performance
Multilayer Perceptron (MLP)	1. Simple and effective for low-complexity tasks with fast training and evaluation. 2. Can handle nonlinear input–output mappings. 3. Scales well with moderate dimensionality.	1. Simple architecture ensures ease of training and interpretation. 2. Good baseline model for testing feasibility and low-dimensional problems. 3. Requires fewer computational resources. 4. Allows rapid exploration of parameter space.	1. Requires hyperparameter tuning to avoid overfitting. 2. Struggles with high-dimensional inputs compared to advanced architectures. 3. Struggles with capturing spatial correlations (consider CNNs). 4. Lacks inherent physical constraints (consider PINNs).	**39** single-functional metasurface units are generated in under 2 s [95].
Tandem Neural Network (TNN)	1. Handles complex non-linear relationships and multi-objective optimization problems. 2. Allows modular design and integration of different MLPs for specific tasks. 3. Can be used for both forward and inverse modeling.	1. Excels in learning from large and unstructured datasets. 2. Addresses degeneracies in inverse design tasks, enabling accurate mapping from target responses to designs. 3. Resolves ambiguity in mappings.	1. Requires significant computational resources for pretraining. 2. Performance heavily depends on dataset quality and task-specific fine-tuning. 3. Post-processing may involve combining outputs from different MLPs or further processing with other models.	<1% relative error in energy ratios achieved using nonlocal acoustic metasurfaces for multichannel wave control [105].
Convolutional Neural Network (CNN)	1. Extracts spatial patterns and features effectively. 2. Suitable for image-like or spatially structured data.	1. Captures spatial correlations and local features effectively. 2. Powerful for topology optimization. 3. Handles complex unit cell geometries. 4. Robust to small variations in input images.	1. Requires significant computational resources for training. 2. Struggles with non-Euclidean geometries. 3. Interpretability can be challenging.	**97%** ultra-broadband sound absorption achieved in the 860–8000 Hz range [91].
Autoencoder (AE)/Variational Autoencoder (VAE)	1. Learns compact representations of high-dimensional data. 2. Can generate new designs by interpolating latent space. 3. Provides uncertainty quantification.	1. Efficient for high-dimensional design spaces. 2. Enables smooth interpolation between designs (VAEs). 3. Useful for data compression and denoising. 4. VAEs offer a probabilistic framework for design generation.	1. Limited scalability for extremely complex geometries. 2. Information loss during encoding. 3. VAEs can generate blurry or less realistic designs compared to GANs/diffusion models. 4. Latent space interpretation can be challenging.	**100** anechoic coating topologies were generated in approximately 3 s, with enhanced design efficiency and accuracy [137].
Generative Adversarial Network (GAN) (Unconditional & Conditional)	1. Generates realistic and diverse samples even with limited labeled data. 2. Enables creative generation for underexplored material design spaces.	1. Explores large design spaces effectively. 2. Can generate novel designs. 3. Useful for discovering new design concepts. 4. cGANs enable targeted design generation and provide control over generated properties.	1. Training instability and difficulty in controlling generated properties (especially in unconditional GANs). 2. Evaluation of generated designs can be challenging. 3. Mode collapse can limit design diversity.	Real time hologram reconstruction with a state-of-art peak signal-to-noise ratio of **24.05dB** [138].
Reinforcement Learning (RL)	1. Learns directly from interaction with the environment, optimal for sequential decision-making problems. 2. Handles complex design spaces and multi-objective optimization. 3. Adapts to dynamic environments.	1. Suitable for tasks involving sequential decision-making. 2. Effective for complex multi-step optimization tasks because it can adapt to new objectives via reward shaping.	1. Performance depends on the reward function's definition and the quality of the simulated/real environment. 2. Training is computationally expensive. 3. Convergence is not guaranteed.	Enhanced underwater coating loss prediction (0.026%, 0.33% error) using 100,000 samples and 20 parameters [139].
Physics-Informed Neural Network (PINN)	1. Combines data-driven learning with physical laws which further reduces reliance on large datasets. 2. Prediction of target properties and field variables, which can solve both forward and inverse problems.	1. Enforces physical consistency. 2. Reduces training data requirements which enables solving multi-physics problems that can be used for parameter identification and model calibration.	1. Complex model architecture. 2. Requires domain expertise in the underlying physics. 3. Training can be challenging for complex PDEs.	Achieves <1% error in predicting parametric acoustic metastructures, considering both explicit and implicit parameters [135].

by learning complex distributions, enabling efficient exploration of the design space. RL offers a robust framework for tackling complex inverse design problems, especially those requiring sequential decision-making in high-dimensional design spaces. These seven ML algorithms provide versatile tools to address diverse inverse design challenges in phononics. Table 3 provides a comprehensive evaluation of these ML models

for metamaterial design, highlighting their unique capabilities, challenges, and some demonstrated performance. Compared to traditional approaches like genetic algorithms and level set methods, ML models offer substantial improvements in efficiency, scalability, and the ability to manage complex relationships. However, these methods are data-intensive and often struggle with generalization and interpretability, which present ongoing challenges for the future of ML in phononic metamaterial design. These algorithms primarily rely on statistical and regression techniques to extract patterns from data [140], correlating input parameters with output responses.

While ML has proven highly effective in many fields, its performance in physics and materials science has been still less promising. These domains often involve problems that require precise solutions through partial differential equations (PDEs) and numerical methods such as the FEM and boundary element method (BEM). These classical techniques remain essential for the design of PnCs and AMs/EMs due to their superior accuracy. However, as discussed earlier, the rise of PINNs is beginning to bridge the gap between ML and physics-based modeling. PINNs integrate physical laws directly into neural networks, reducing the need for large datasets while improving accuracy, generalization, and convergence speed. Their ability to solve PDEs and other physics-related problems has drawn significant attention for inverse design tasks, offering data-efficient and physically consistent solutions [141]. While PINN-based methods still face significant challenges in efficiently handling complex, large-scale and high-dimensional problems [142], especially in the field of AMs/EMs where their use is scarcely reported, they offer two critical features that benefit inverse design: physics-awareness and differentiability.

Physics-awareness, though not strictly necessary for inverse design, is highly advantageous as it generally reduces the size of the training dataset required. Furthermore, physics-aware models exhibit superior extrapolation capabilities compared to purely data-driven approaches, enabling the search for optimal designs beyond the initial dataset. While PINNs are inherently physics-aware, it is possible to integrate physics-awareness into other architectures, such as VAEs. For instance, a vanilla VAE trained on unit cells of a specific types demonstrates limited understanding of acoustic or mechanical properties, simply due to the existence of direct property-geometry relationships. Latent spaces optimized purely for geometric reconstruction may struggle to generate desired behavior, such as bandgaps, particularly in cases where acoustic phenomena are highly sensitive to geometric variations. Recent works on mechanical metamaterials [143,144] have shown that introducing an auxiliary property predictor acting on the latent space can significantly reorganize it, making the space property-aware. Additionally, splitting encoders and decoders to separately encode geometry and properties into the same latent space has proven effective in disentangling geometric and material components of the latent vector.

However, achieving robust physics-aware frameworks for inverse design in some cases can be hindered by fundamental limitations in generative architectures themselves, particularly when applied to metamaterials. Many generative models, initially designed for image processing, struggle to operate effectively in poorly structured design spaces. Unlike the image domain, which is inherently continuous and topologically well-defined (allowing valid interpolation between images) [52], metamaterials often impose additional geometric constraints, such as the absence of topologically separated components. If these constraints are simple and can be manually implemented by limiting the range of design parameters, classical generative models have been shown to succeed in generating structures similar to those in the training dataset [143,145]. However, more complex restrictions required for certain classes of metamaterials can hinder the ability of classical generative models to operate in topologically disconnected direct spaces or to learn mappings to a well-structured latent space [146]. This is a known issue in computer science, particularly in the field of constraint learning [147], and it make whole families of metamaterials almost unachievable for ML-based inverse design. In general, a well-structured latent space containing maximally disentangled information about geometry and properties can be explored using tools like t-Distributed Stochastic Neighbor Embedding (t-SNE) [148,149], Uniform Manifold Approximation and Projection (UMAP) [150,151] or SHapley Additive exPlanations (SHAP) [152]. Such latent space is not only facilitates the creation of interpretable and explainable models but also accelerates optimization and the search for designs beyond the initial dataset. This represents a clear direction for the future, which, to our knowledge, is still barely explored in the domain of AMs and EMs. Achieving robust and scalable physics-aware frameworks for inverse design remains a critical challenge for advancing the development of AMs and EMs.

The inverse ML methods discussed in this review are often applied to facilitate inverse design at the unit cell level, assuming that the entire metamaterial or phononic crystal is constructed by repeating such unit cells in two or three dimensions. This approach ensures relatively low dimensionality of the geometry space while maintaining sufficient variability in properties, especially those influenced by the periodicity of the structure, such as Bragg-scattering bandgaps. However, current trends toward heterogeneous [153] or even aperiodic [154] architectures, which combine unit cells of different geometries, necessitate modifications to these methods. In such cases, the goal of inverse design shifts to identifying a set of unit cells that, when assembled, deliver the desired performance, such as wave steering [103]. In specific scenarios, where each unit cell is chosen from a limited number of options, the entire metamaterial can be represented as a pixel-like image, enabling the direct training of classical mechanical models on the entire metamaterial [153] However, more commonly, models trained at the local (unit cell) level must be integrated with optimization processes operating on a global scale [95,155]. Gradient-based global optimization could benefit significantly from the elimination of non-differentiable operations, such as finite element (FE) simulations, from the optimization loop. Physics-informed neural networks satisfy this requirement, but they might struggle when addressing non-linearities, such as those associated with viscoelasticity [156]. Employing for this task surrogate models [157] or incorporating automatic differentiation [158] seems feasible, but achieving robust differentiability across multi-scale, multi-physics systems remains an open challenge. Progress in this area could unlock new opportunities for efficient inverse design in PnCs and AMs/EMs.

Regardless of whether the inverse approach is purely data-driven or incorporates physics-aware aspects, the initial dataset plays a crucial role in the subsequent training and performance of the model. Generating a huge and versatile dataset through rigorous analytical models, numerical simulations, and extensive experimental tests can be highly computationally intensive and time-consuming which raises concerns about the overall efficiency and feasibility of data-driven methods. This challenge is partially reduced by using transfer learning [141] and data augmentation [159]. Also, various sampling techniques such as Monte Carlo sampling and SOBOL sequences can be employed to select optimal sample size which reduces the computational burden and improves the efficiency of the data generation process [160]. By strategically sampling the input space, these techniques ensure that the data used for training is both representative and sufficient, thus enhancing the performance of the ML models without incurring excessive computational costs. Multimodal LLMs can also help here. These models represent a significant advancement in ML and offer a versatile foundation for a multitude of tasks. With the collective efforts of the phononic community, vast amounts of experimental and simulation data of phononic designs (including structure, material properties, and its behavior under various conditions) can be gathered. Techniques such as transfer learning and data augmentation can be employed to reduce data requirements, enhance generalization, and accelerate the design process. Developing a generalized model specifically tailored for phononic metamaterials can offer substantial benefits by providing advanced insights, guidance, and analysis capabilities for professionals working in this field.

A fundamental limitation of using generative ML approaches in the design of metamaterials for real-life applications is the lack of uncertainty or sensitivity quantification in most common methods. The majority of generative models simply provide the resulting geometry. However, in real-world scenarios, any measured property is characterized not just by a single value but by two values: mean and variance. Therefore, it is crucial to gradually transition from deterministic models to Bayesian approaches—a shift that has already begun [161,162]. Bayesian approaches not only provide uncertainty quantification but, when coupled with underlying models such as Gaussian Processes, enable more efficient exploration of the design space compared to the typically random generation of the training set [163]. Even within the deterministic paradigm, sensitivity can be addressed by enforcing solutions that are less sensitive to changes in input parameters [164–166]. If such measures can be implemented in machine learning algorithms [167], future models might demonstrate much better acceptance in the design and manufacturing of metamaterials.

Finally, advancements in manufacturing techniques and engineering have led to the emergence of elastic and acoustic metamaterials that are no longer "frozen in time and space" [168]. These so-called active, tunable, or reconfigurable metamaterials can modify their effective performance through, for instance, changes in their internal geometry triggered by external stimuli [169]. Furthermore, advanced AMs/EMs are increasingly being designed to perform multiple functions simultaneously, as demonstrated in acoustoelastic metamaterials [170]. Recently, a metamaterial capable of focusing elastic waves at different locations depending on the applied compressive strain was introduced [158]. For such a complex task, classical optimization methods with automatic differentiation were employed, as machine learning approaches were not yet suitable. To remain useful, machine learning-based design methodologies must adapt to accommodate the multi-objective design challenges arising from these new metamaterials.

To overcome all the above-mentioned obstacles, a universal framework of methods and architectures that enables more efficient and versatile metamaterial design must be developed. Obtaining databases of unit cells [171], a set of machine learning [172] and classical optimization [173] approaches, and fabrication tools [174] is not enough unless all these components work in synergy. A recent attempt to create the so-called phononic structures genome engineering (PSGE) [175] seems promising. At the same time, it requires organized and continuous contributions from multiple groups and individual researchers.

Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this work the authors used ChatGPT in order to make final english proof-reading. After using this service, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

Partially funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy – EXC-2193/1 – 390951807.

Appendix. Glossary

- **Artificial Intelligence** is the overarching discipline encompassing algorithms and computational techniques aimed at simulating or surpassing human cognitive functions, including learning, reasoning, and decision-making. AI encompasses techniques like machine learning, natural language processing, and computer vision.
- **Machine Learning (ML)** is a subset of artificial intelligence that enables systems to learn patterns from data and make predictions or decisions without being explicitly programmed. It involves training algorithms on datasets to generalize and perform tasks such as classification, regression, or clustering.
- **Neural Network (NN)** is computational model inspired by the human brain, consisting of interconnected layers of nodes (neurons) that process data and learn patterns. These networks can model complex, non-linear relationships between inputs and outputs.
- **Convolutional Neural Network (CNN)** is a specialized neural network architecture designed to process and recognize patterns in data with a grid-like topology (e.g., images), using convolutional and pooling layers. CNNs excel in learning spatial relationships within complex metamaterial unit cells or microstructures, making them suitable for tasks such as topology optimization and fast geometry-to-property mapping.
- **Convolutional Layer** is an component of CNN that applies convolution operations to input data, extracting spatial features such as edges, textures, or patterns by using learnable kernels.
- **Pooling Layer** is an component of CNN that reduces the spatial dimensions of the data by summarizing local regions to reduce computational complexity and prevent overfitting.
- **Supervised Learning** is a type of ML where the model is trained on labeled data, learning to map inputs to outputs based on presented input–output pairs. Supervised Learning is often used to predict metamaterial properties (e.g., bandgaps) from known structural parameters,
- **Unsupervised Learning** is a type of ML where the model identifies patterns or structures in unlabeled data without predefined outputs. Unsupervised Learning is often used in clustering or discovering new metamaterial designs with similar acoustic or elastic properties, even when labeled data is unavailable.
- **Reinforcement Learning (RL)** is a type of ML where an agent learns to make decisions by interacting with an environment and receiving rewards or penalties. RL can optimize metamaterial designs by iteratively adjusting parameters to achieve desired wave manipulation properties.
- **Transfer Learning** is a ML technique where a pre-trained model is adapted to a new, related task, reducing the need for large datasets. Transfer Learning enables the reuse of ML models trained on similar problems to accelerate the design of new metamaterials, saving computational resources.
- **Active Learning** is a ML approach where the model iteratively selects the most informative data points to be labeled and added to the training set, rather than using a static dataset. Active learning optimizes the design of acoustic and elastic metamaterials by focusing computational resources on the most critical simulations or experiments.
- **SOBOL Sequence** is a quasi-random sampling method used to ensure uniform coverage of the design space with fewer samples compared to random sampling, enabling more efficient exploration of high-dimensional parameter spaces.
- **Discriminative Model** is a model that focuses on learning the boundary between different classes or the mapping from inputs to target labels. It uses training data to directly estimate how likely an input belongs to each possible output category or continuous value. Discriminative models are commonly used to map metamaterial geometric parameters to their corresponding properties.

- **Generative Model** is a model that attempts to learn the underlying distribution that produced the observed data. By capturing this distribution, it can generate new, realistic samples that share statistical properties with the training set. Generative models can produce new metamaterial designs that are likely to exhibit desired acoustic or elastic performance.
- **Latent Space** is a lower-dimensional representation of data where essential features are captured and encoded into compact form, often used in generative models. Latent space simplifies the exploration of complex metamaterial design spaces, enabling efficient optimization and generation of novel structures.
- **Training** is the process of teaching a ML model to make accurate predictions by adjusting its parameters based on a dataset. It involves minimizing a loss function through iterative optimization algorithms like gradient descent.
- **Loss function** is a mathematical function that measures the difference between a model's predictions and the actual target values, guiding the optimization process during training.
- **Overfitting and underfitting** represent two extremes of model complexity, with overfitting demonstrating excessive variance and underfitting characterized by high bias. Overfitting arises when a model memorizes training data, including noise and outliers, and thus fails to generalize to new cases, whereas underfitting stems from a model that is too simple or insufficiently trained to capture essential patterns.
- **Regularization** is a technique used to prevent overfitting by adding a penalty term to the loss function, discouraging overly complex models.

Data availability

No data was used for the research described in the article.

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