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Review

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Machine learning assisted intelligent design of meta structures: a review

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Abstract

In recent years, the rapid development of machine learning (ML) based on data-driven or environment interaction has injected new vitality into the field of meta-structure design. As a supplement to the traditional analysis methods based on physical formulas and rules, the involvement of ML has greatly accelerated the pace of performance exploration and optimization for meta-structures. In this review, we focus on the latest progress of ML in acoustic, elastic, and mechanical meta-structures from the aspects of band structures, wave propagation characteristics, and static characteristics. We finally summarize and envisage some potential research directions of ML in the field of meta-structures.

Keywords: Meta-structure, inverse design, machine learning, continuous fiber reinforced composite meta-structure, additive manufacture

INTRODUCTION

Meta-structures[1] are artificially designed functional structures that meet specific performance requirements and possess physical properties beyond the capabilities of natural materials. Based on different disciplines, acoustic meta-structures[2], mechanical meta-structures[3], electromagnetic meta-structures[4], and other types can be distinguished. Acoustic meta-structures[5], including phononic crystals, acoustic metamaterials, and acoustic metasurfaces, have emerged as an elegant means of manipulating acoustic and elastic waves. Through special structural designs, researchers can achieve dynamic characteristics that are not found in natural materials, enabling novel operations such as mechanical wave blocking[6], absorption[7,8], focusing[9,10], robust energy harvesting[11,12], negative refraction[13], invisibility[14,15], topological transmission[16], and more. The significant advancement in the field of acoustic meta-structures can be attributed primarily to the extensive research conducted on electronic crystals and photonic crystals. Matter waves and electromagnetic waves exhibit band structures separated by bandgaps under the action of Bloch periodic potential fields formed by the above structures. Bandgap formation is attributed to the Bragg scattering mechanism, which results from destructive interference between scattered waves caused by periodic structures. Phononic crystals[17,18], which are formed by the periodic distribution of materials or structures in space, can exhibit bandgaps that effectively block or attenuate the propagation of mechanical waves as an extension of the aforementioned concept. The subsequent development of localized resonant phononic crystals enables the formation of low-frequency hybridization bandgaps through scatterer resonance, independent of the periodicity of the structure itself[19]. The local resonance mechanism has triggered a revolutionary innovation in the realm of acoustic metamaterials[20]. On the one hand, the bandgap frequency is determined by the resonant unit frequency, providing theoretical support for developing compact structures with vibration and noise reduction functions in limited space requirements. On the other hand, it has been proven to possess new physical properties with locally resonant parameters, resulting in equivalent excotic properties. This has stimulated extensive research on negative mass density[21], negative bulk modulus[22,23], and double-negative parameters[24,25].

In the past decade, guided by the goal of achieving efficient regulation of low-frequency acoustic/elastic waves through thin and lightweight structures, researchers have developed acoustic metasurfaces by designing subwavelength functional unit arrays to form phase gradients based on the generalized Snell's law[26]. Acoustic metasurfaces[27] include reflective, absorptive, and transmissive types, which can achieve functions such as acoustic/elastic wave focusing[28], cloaking[29,30], low-frequency perfect absorption[31,32], asymmetric transmission[33], self-bending[34], and so forth. Compared with phononic crystals and acoustic metamaterials, acoustic metasurfaces have the characteristics of ultra-thin, planar, low loss, and strong designability, which make it possible to develop extremely miniaturized acoustic functional devices.

Recently, the concept of topological insulators in condensed matter physics has been added to the design of acoustic meta-structures for regulating mechanical waves[35-39]. Due to the existence of bandgaps, mechanical waves within specific frequency ranges are not allowed to propagate. In these bandgaps, acoustic meta-structures can be considered as insulators of mechanical waves. The topological properties of bandgaps can be characterized by calculating topological invariants and can generally be classified as topological trivial and topological non-trivial bandgaps[40,41]. On the structural boundaries with the above two bandgaps, certain frequencies of waves within the bandgap are allowed to propagate, which are the so-called topological edge states. Supported by topological mechanisms, topological edge states have robust transmission characteristics, such as defect immunity, unidirectional waveguides, and backscatter suppression effects[42,43]. The in-depth studies of topological states have broadened the application prospects of acoustic meta-structures to a certain extent.

The research on mechanical meta-structures primarily centers around the three material parameters of elastic modulus, shear modulus, and Poisson's ratio in order to attain exceptional static performance[3].

Natural solid materials typically exhibit positive elastic and shear moduli, which are related by Poisson's ratio, typically falling between 0 and 0.5. The mechanical meta-structures designed through origami and kirigami structures[44], chiral structures[45], lattice structures[46], honeycomb structures[47], and other methods can constrain and adjust the overall elastic deformation, thus exhibiting unconventional equivalent characteristics, such as negative stiffness, negative compression, negative Poisson's ratio, multi-stability, and so forth. Mechanical meta-structures greatly enrich the way of regulating statics performance and provide support for the design and application of engineering vibration suppression, impact resistance, energy absorption, and structural protection devices.

The process of analyzing the wave or mechanical properties of a certain meta-structure is a forward problem, which can be easily realized through theoretical, experimental, or commercial software analysis. However, designing structures with specific properties considering practical application backgrounds can essentially be attributed to inverse problems[48]. The traditional strategy for solving inverse problems usually relies on trial and error supported by experimental and computational modeling techniques, which require a significant amount of time and resource costs. Subsequently, some heuristic optimization methods that relied on global search were developed, such as genetic algorithms (GA)[49], simulated annealing algorithms[50], particle swarm optimization algorithms[51], and so forth. These methods can effectively identify the meta-structure parameters corresponding to the target property and can be modified to adapt to different goals. However, their performance generally depends on the specific problem, usually lacking stability and being prone to falling into local optima.

With the deepening of artificial intelligence (AI) research, the improvement of computer hardware performance, and the emergence of open-source deep learning frameworks, machine learning (ML) algorithms have been rapidly developed and widely applied, and advanced methods, such as deep neural networks (DNNs) and reinforcement learning (RL), have emerged. The development of ML has shown a strong ability to circumvent the shortcomings of traditional methods, leading to an interdisciplinary revolution, including biology[52], finance[53], materials science[54], computational chemistry[55], computational mechanics[56], *etc.* Certainly, the meta-structure design scheme based on intelligent algorithms has become an important core to break through the bottleneck of inverse problems and promote the development of the field. In the past several years, some review articles have introduced the latest progress of ML-enabled meta-structure design from different aspects, for instance, the progress of ML-enabled nanophotonics and photonic devices in an all-round way[57-66]. Furthermore, Khatib *et al.* introduced the progress in the field of designing electromagnetic meta-structures by ML[67]. Jiao *et al.* discussed the advent and prospects of ML in the field of mechanical meta-structures[68]. Jin *et al.* introduced some basic ML algorithm principles and reviewed intelligent on-demand design of phononic metamaterials[69]. Subsequently, Muhammad *et al.* and Liu *et al.* successively updated the progress of ML in phononic crystals and metamaterial[70,71]. From the works in recent years, the field of integrating ML in the design of acoustic, elastic, and mechanical meta-structures has developed rapidly, but there is still a lack of comprehensive review that directly takes design objectives as the classification standard, which is helpful to understand the latest progress of various inverse design problems in this field.

In this review, we draw attention to a series of recent results on ML inverse design of acoustic, elastic, and mechanical meta-structures from the perspective of design objectives. We first introduce the background of the development of ML and how basic algorithms can be combined with meta-structures for inverse design. Then, we summarize the latest progress from three aspects: design of band structure in infinite meta-structures, design of wave propagation characteristics in finite meta-structures, and design of static characteristics in mechanical meta-structures. Finally, we summarize the current status of this cutting-edge cross-disciplinary field and discuss potential future development prospects.

BACKGROUND OF ML

AI is committed to enabling machines to acquire and expand human intelligence. The development of AI can be traced back to the proposal of this concept at the Dartmouth Conference in 1956, but related research has already begun earlier. It has gone through periods of symbolism, connectionism, and behaviorism[72]. Early researchers constructed expert systems by feeding human experience into machines through programming, which is a symbolic approach. Although expert systems perform well in environments with strong logic, such as mathematical deduction, this approach cannot obtain new knowledge beyond input, and human intelligence is acquired through autonomous learning rather than direct input. Therefore, researchers turned to exploring ways to enable machines to autonomously acquire knowledge starting in the 1980s, a concept known as ML[73]. At this time, connectionism represented by an artificial neural network (ANN) algorithm ushered in the peak of development. Artificial neurons were proposed in 1943[74], followed by the development of a variable strength criterion for inter-unit connections, which led to the formation of a perceptron model[75]. In 1986, the success of the back-propagation training algorithm enabled the multilayer perceptron (MLP) model to have nonlinear processing capability[76]. On this basis, researchers began to explore the deepening of neural network models. Recurrent neural networks (RNN)[77] with time series prediction function and convolutional neural networks (CNN)[78] with image processing function were successively proposed. The deepening of the model has brought about an explosive increase in training difficulty, but this dilemma has been effectively overcome with the improvement of computer computing power. Since 2006, research on ANNs has entered the era of deep learning[79], and the emergence of many open-source deep learning frameworks has greatly reduced the learning cost of algorithms. Over the past decade, a large number of DNN models have emerged, such as generative adversarial networks (GAN)[80], condition GANs (CGAN)[81], tandem neural networks (TNN)[82], and so forth. RL, originating from behaviorism[83], has gradually emerged in the context of the flourishing development of deep learning. The basic principle is that the agent takes different actions to change its own state and corrects its behavior based on environmental feedback, thereby selecting the optimal strategy to achieve the goal. RL is seen as the future development direction of AI and has achieved great success in fields such as Go programs[84] and autonomous driving[85].

The advantage of DNNs lies in their ability to learn potential laws implicitly from data, especially for nonlinear mapping problems with unclear or complex physical mechanisms, and the design of meta-structures belongs to such problems. Unlike the process of calculating property from structural parameters in a forward problem, inverse design, which involves extrapolating the property back to the structure, often finds it difficult to obtain analytical solutions based on clear functional relationships. However, with the nonlinear processing ability of data-driven neural networks, the design parameters of the structure can be quickly obtained by taking the target property as input.

For situations where high-dimensional data or image data are used as property inputs, CNNs are often used to reduce the number of connections between neurons, thereby reducing the computational complexity of the computer. Autoencoders (AE) can be used to extract features from high-dimensional property data for further wave or mechanical analysis. In the inverse design meta-structure paradigm, there may be a problem that one property corresponds to multiple sets of structural parameters, which leads to the convergence failure of neural network training.

The proposal of TNN effectively solves this problem by freezing the training parameters of the pre-trained forward network and cascading it after the inverse network[82]. The subsequently developed probabilistic

TNN can obtain multiple reasonable structures as alternative solutions based on inputs. Additionally, in order to deal with the situation of only small-scale data, researchers introduced transfer learning into meta-structure design[86,87]. Transfer the model trained from similar data sources to the target data for retraining, thereby reducing the demand for target data without affecting the training results.

Another solution is to rely on GAN[80] and CGAN[81]. In this solution, the generator of GAN takes random vectors as input, initiates the generation of a structure, and then sends the generated structure and real structure to the discriminator for authenticity discrimination to guide model updates. After adversarial training of the generator and discriminator, a generator model that can generate the target structure can be obtained. While inputting random vectors, the expected property can be input together to enable the generator to generate structures under this condition. The combination mode of RL and meta-structure inverse design is to regard structural parameters as agents. These agents execute the action of parameter changes, determine feedback based on the proximity of the altered property to the design goal, and finally explore a parameter path to achieve the goal.

As a summary, the overview diagram of ML in the field of meta-structure for forward performance prediction and inverse structure design is shown in Figure 1. In addition, there are various types of ML algorithms, some of which may be simple and perform well when dealing with specific problems. For example, linear regression obtains sample distribution patterns by fitting data points as closely as possible. Logistic regression can compress samples to a specific range through nonlinear functions, thus realizing the classification of samples. A decision tree is a tree-structured classifier that classifies samples by representing branches of different attributes. Multiple groups of decision trees can form a random forest, which yields higher performance and prediction stability. However, the increase in the complexity of the model requires more computing time. Readers can refer to relevant literature for more information[73,88,89].

The emergence of some deep learning open-source frameworks, such as TensorFlow[90] and PyTorch[91], helps beginners easily grasp the basic usage of ML. These frameworks are integrated through Python packages and can be easily called, eliminating the hassle of writing low-level computational code for neural networks. Researchers can use some shared ready-made datasets for training and learning, such as Handwritten Digit Dataset, CIFAR10, Fashion-MNIST, and so forth. In addition, the commercial software MATLAB also has a built-in toolbox for neural networks, which can be easily modeled through the user interface.

APPLICATION OF ML IN META-STRUCTURES

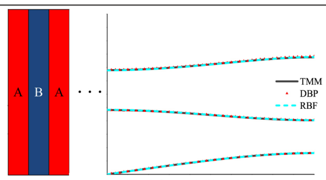
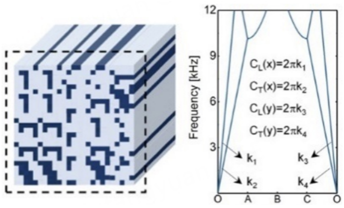
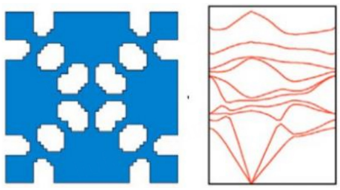
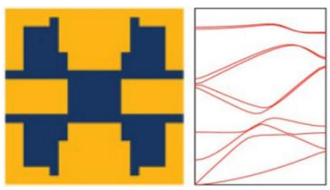
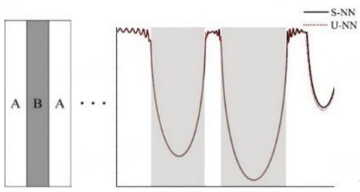
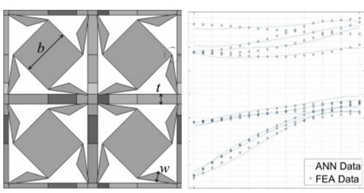
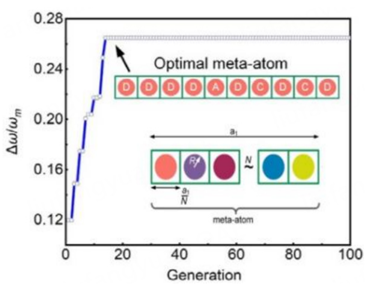
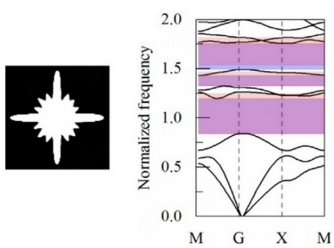
Design of band structure in infinite meta-structures

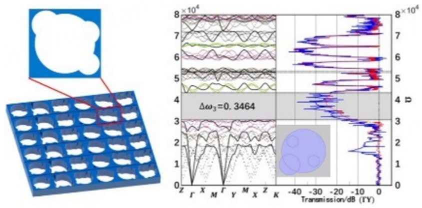
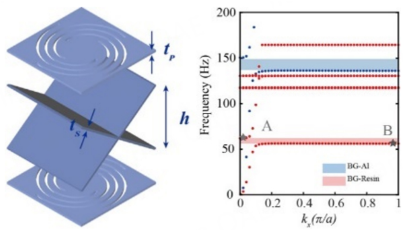
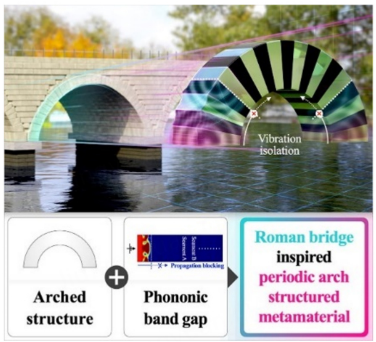
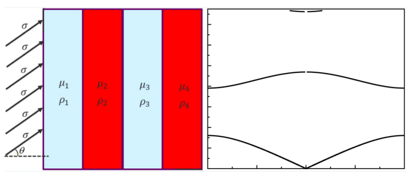
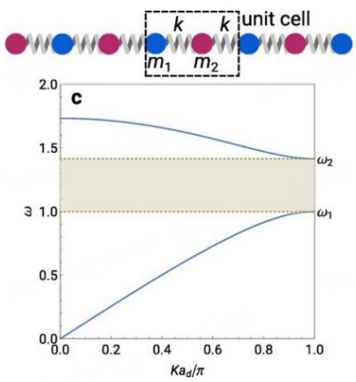
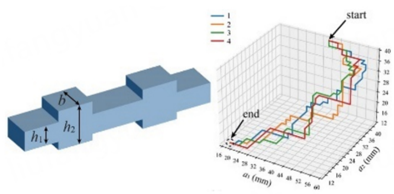
A band structure is the most basic way to describe the acoustic/elastic wave characteristics in meta-structure, so it is the most direct research idea to carry out the application of ML in meta-structure design around a band structure and the wave information it carries. With the maturity of deep learning algorithms and open-source frameworks, a large amount of design work has emerged around band structures, which can be mainly divided into two categories: design based on complete band structures and design based on bandgaps. Table 1 provides a brief overview of ML for the design of band structures in infinite meta-structures.

Complete band structures

For the design of complete band structures, one type of work is to predict the corresponding band structure of a meta-structure from a forward perspective to replace the analytical process. Liu and Yu[92] used MLP and radial basis function neural networks (RBF-NN) to predict the band structures of one-dimensional

Table 1. A brief overview of design based on band structures in infinite meta-structures

Design type	Algorithm	Meta-structure and performance	Description	Year
Complete band structures	MLP RBF-NN		RBF is suitable for single parameter prediction, while MLP can meet multi-parameter prediction[92]	2019
	CNN		Construct digital structure genomes through forward prediction. Thus, the target property structures can be quickly extracted from the genomes[93]	2021
	GAN CNN		Generate optimal structure based on customized dispersion and accelerate design processes[94]	2022
	GAN CNN		Generate and screen structures with excellent attenuation performance. The dataset is generated through secondary mirroring, which lacks flexibility[95]	2022
Tailoring bandgaps	MLP TNN		Compared to MLP, TNN can solve the problem of data inconsistency and is suitable for multi-parameter inverse design[96]	2019
	GA MLP		The model is insufficient to provide accurate predictions beyond the training data range and only performs well within local data points[97]	2020
	GA MLP		The model can obtain the target modular metamaterial but cannot find the configuration beyond the dataset[98]	2020
	AE MLP		Can accurately process data beyond the dataset. Only a relatively small region of the design space in RVE is explored using a nine-parameter analytical function[99]	2020

GA MLP		Fast forward search to obtain the maximum bandgap structure. Performed well in both single-objective and multi-objective optimization designs[100]	2021
MLP		Flexible design of meta-structures based on target bandgap for vibration isolation. The designed structure has been experimentally verified[101]	2022
TNN		Arch-shaped vibration isolation structure inspired by the Roman Bridge. The TNN model can design structure accurately based on target bandgaps and verified through experiments[102]	2022
RL		Efficient interactive inverse design for layered phononic crystals. For the same model, simply changing the objective function can easily achieve different designs[103]	2020
RL GA		Designing one-dimensional diatomic and hexatomic lattice chains based on RL. The rate of convergence is much faster than the baseline GA[104]	2021
RL		Designing a one-dimensional phononic beam based on RL. The model still maintains an efficient and stable exploration ability in the huge parameter space[105]	2022

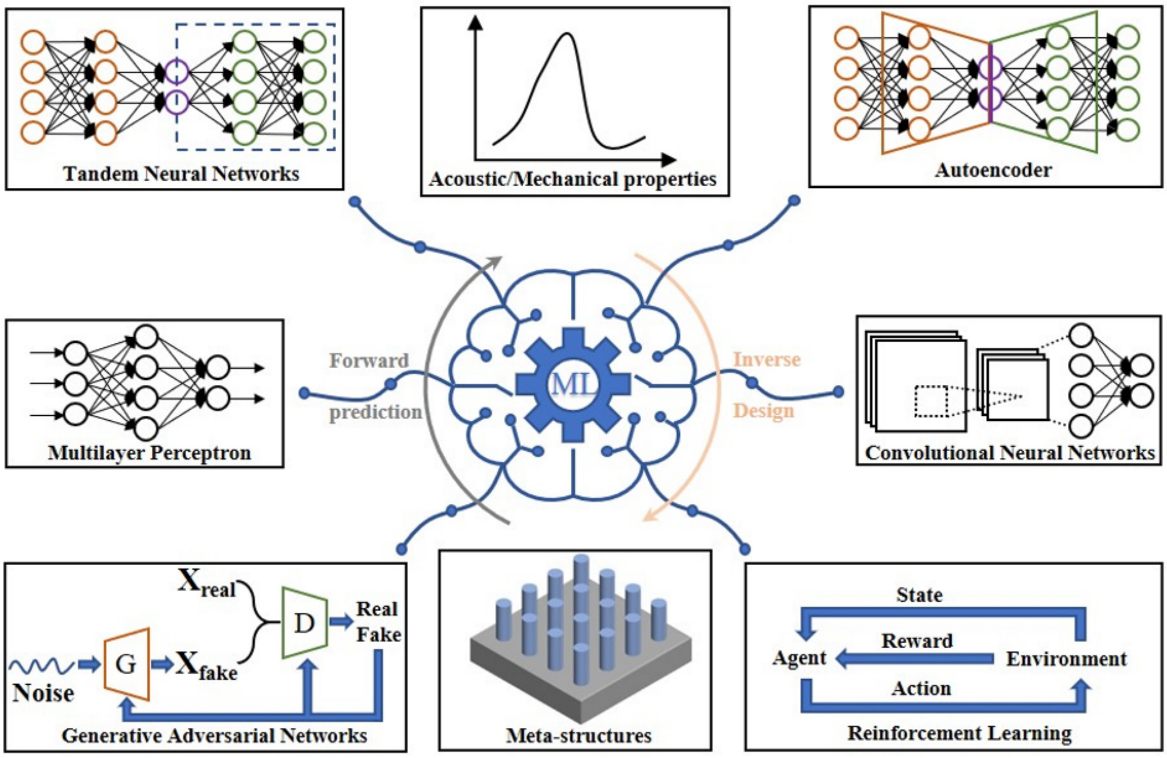


Figure 1. ML in solving the problem of properties prediction and inverse design for meta-structures.

layered phononic crystals and compared their efficiency and accuracy. The input parameters of the neural networks are one to three selected from the filling fraction, mass density ratio, and shear-designed structure. The accuracy in predicting band structures is achieved using a single parameter (fill fraction), while in the case of multiple parameters, MLP outperforms RBF-NN.

Another type of work is to use trained forward models to assist in the selection of alternative structures after inverse design. Zhang *et al.* constructed a digital structural genome using CNN to achieve structural screening with specified elastic wave properties[93]. For representative volume elements (RVEs) of size 5 × 5, each unit has two coding forms, with a total of 2^{25} possible configurations, which makes it difficult to find configurations with target elastic wave properties. Their approach is to calculate the band structures of a small portion of RVEs using a finite element method and extract wave properties to construct a dataset. Then, by using data-driven CNN to predict the elastic wave properties of all possible configurations, a digitally structured genome is constructed. For a set of target elastic wave properties, the corresponding structure can be found in the genome. Jiang *et al.* proposed a novel way to inverse design similar digitally coded metamaterials, as shown in Figure 2A[94]. This work can be divided into three steps: first, train CNN to predict the band structures; second, train GAN to generate digitally coded metamaterials from band structures; and finally, take out the generator of GAN and connect it with CNN. The overall workflow is as follows: the generator takes random noise and target band structures as inputs, generating a series of alternative structures. Predict the corresponding band structures of all candidate structures through CNN and then compare them with the target band structure to screen the best structure. Almost at the same time, Han *et al.* employed the same design process to realize inverse design of digitally coded metamaterials with

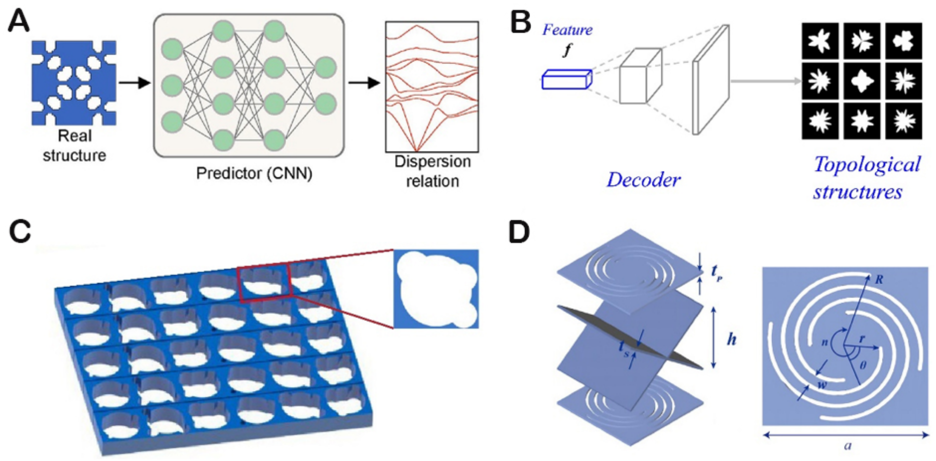


Figure 2. ML for the design of band structure in infinite meta-structures. (A) Combining GAN and CNN to realize inverse design of digitally coded metamaterials with anticipated band structures[94]. Reproduced with the permission of Ref.[94] Copyright 2022, Elsevier. (B) Design phononic crystals with anticipated bandgaps by combining AE and MLP[99]. Reproduced with the permission of Ref.[99] Copyright 2020, Elsevier. (C) Design phononic crystals with anticipated bandgaps by combining GA and MLP[100]. Reproduced with the permission of Ref.[100] Copyright 2023, Taylor & Francis. (D) Employ MLP to design lightweight meta-structures with low-frequency broadband vibration isolation functions[101].

optimal wave attenuation[95]. It is worth noting that this work characterizes the wave attenuation ability of the structure through complex band structures. Although the design process focuses on the real part of the band structures, the final screening process from alternative structures is achieved by comparing the imaginary part of band structures.

Tailoring bandgaps

From an application perspective, it is usually not necessary to determine the complete band structures but only focuses on the wave information provided by the bandgaps in the band structures. In contrast, the design based on bandgaps simplifies the difficulty of model training and has a stronger design purpose, so a lot of work has been carried out in this area.

Liu *et al.* employed MLP and TNN to achieve inverse design from bandgaps to structures for the layered phononic crystals[96]. The basic conclusion is that for inverse design with single (filling fraction) or dual (shear modulus ratio and mass density ratio) parameters, MLP and TNN perform equally. However, for inverse design with three parameters, TNN has obvious advantages, while MLP has difficulty in convergence. This is due to the increase in the number of design parameters deepens the nonlinearity of the mapping, leading to the gradual exposure of data inconsistency issues. As mentioned in the introduction, TNN can effectively solve this training bottleneck. Dong *et al.* proposed using GA to optimize MLP architecture for fast prediction of bandgap width[97]. The starting point of this study is to serve as an efficient means to avoid the significant computational costs required for repeated finite element analysis of elastic meta-structures. Wu *et al.* explored a design and optimization scheme of modular metamaterial using ML[98]. In their work, modular metamaterials are composed of a certain number of four candidate materials through different configurations to form phononic crystals. By using GA and MLP, they realize the optimal configuration design of one-dimensional and two-dimensional (2D) modular metamaterial according to the bandgap target. Li *et al.* combined an AE with MLP to achieve 2D phononic crystal design with anticipated bandgaps, as shown in Figure 2B[99]. The RVE of phononic crystals is generated through random functions, and the band structure data are obtained through a finite element method. The implementation of this design consists of three steps. Firstly, the AE is trained to extract the topological features of the RVE configuration. Secondly, an MLP model is trained to describe the relationship between the anticipated bandgap and topological features. Finally, the encoder in the AE is replaced with MLP. Miao *et al.* conducted another study on the design of 2D phononic crystals described by random functions, as shown in Figure 2C[100]. In this work, they first employed MLP to predict the bandgap and then used MLP combined with GA to achieve the inverse design of the structure. In the inverse design scheme, GA is taken as the main body, and the fitness function is constructed with the predicted bandgap of MLP and the target bandgap in the iterative process, and the optimal individual that can adapt to the target bandgap is obtained through iteration.

In terms of meta-structure design with high-quality vibration reduction function, Jin *et al.* employed MLP to inverse design the Archimedes spiral meta-structure with deep subwavelength vibration isolation function, as shown in Figure 2D[101]. The double-layer corrugated core sandwiched structure between two spiral plates can provide low-frequency bandgaps through a local resonance mechanism. However, it is difficult to analyze the relationship between the bandgap and the parameters of the spiral plate. The trained MLP model avoided the analytical process of inverse design and obtained a structure with low-frequency broadband vibration isolation performance, which showed good consistency with the experiment. On *et al.* modified the TNN architecture and realized the design of arch meta-structure with anticipated bandgap vibration reduction function[102]. Specifically, they inverted the pre-trained forward network and inverse design network in traditional TNN, where the input is a structural parameter, while the intermediate layer outputs the bandgap frequency. After training, preserving the inverse network of the backend can achieve the design of bandgap frequencies to structures.

The application of RL in band structures is mainly to maximize the bandgap width or optimize the specific range and focuses on one-dimensional structures with analytical dispersion relation. According to the analytical dispersion relation of layered phononic crystals, Luo *et al.* used RL to optimize the component widths and realized two functions: maximizing the bandgap width and customizing the bandgap range[103]. Wu *et al.* employed RL to optimize the masses of one-dimensional atomic chains to achieve custom bandgaps[104]. He *et al.* analyzed the longitudinal wave dispersion of periodically variable cross-section beams and optimized three length parameters using RL to achieve maximum bandgap width[105].

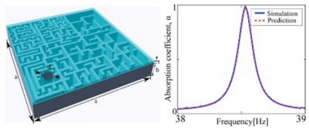
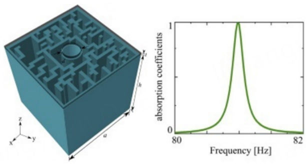
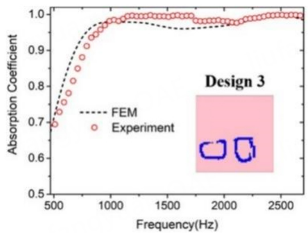
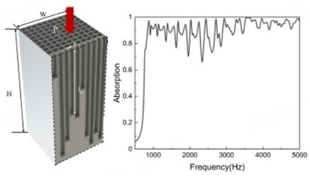
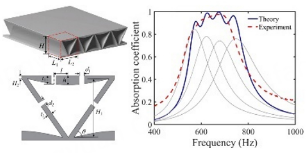
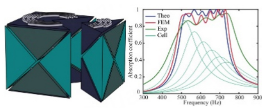
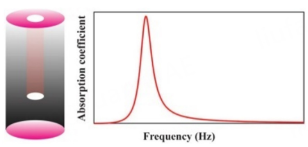
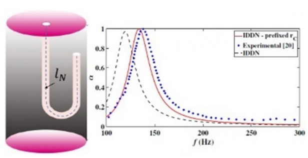
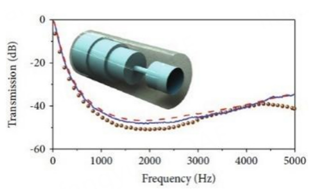
Design of wave propagation characteristics in finite meta-structures

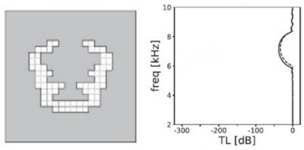
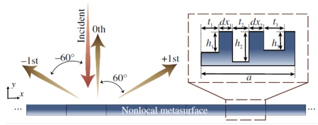
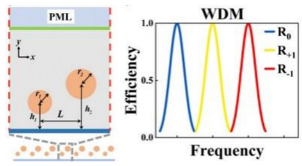
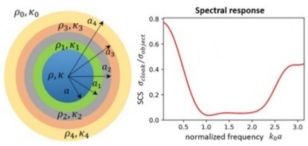
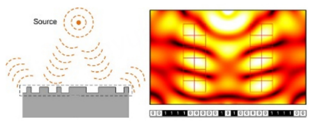
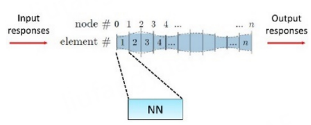
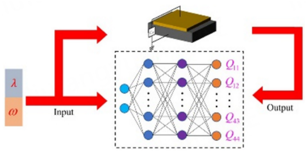
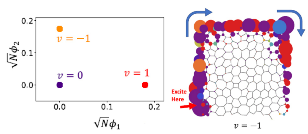
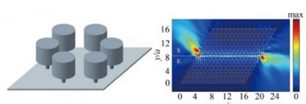
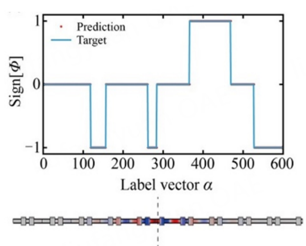
Different from the ideal infinite period meta-structures, the meta-structures in practical engineering can only be composed of periodic or aperiodic finite distributions. Analyzing the propagation characteristics of acoustic/elastic waves in finite meta-structures is an important step toward achieving practical engineering applications for meta-structures. In this section, we review the finite meta-structure design works around propagation characteristics. Table 2 provides a brief overview of ML for the design of wave propagation characteristics in finite meta-structures.

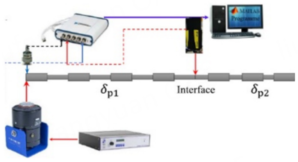
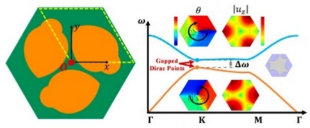
Enhancing noise reduction

Arranging sound absorption structures is one of the main methods for controlling environmental noise, which can be divided into porous sound absorption structures, resonant sound absorption structures, and special sound absorption structures, and has been widely used. The ability of a structure to absorb sound energy is usually characterized by calculating its sound absorption coefficient. Due to the complexity and diversity of the structure, design is an important step to meet practical needs. Researchers have conducted extensive explorations in this area using ML. For example, Donda *et al.* employed CNN to characterize the acoustic absorption performance of acoustic absorbing metasurfaces[106]. Subsequently, they implemented the inverse design of the metasurface using CGAN[107]. Zhang *et al.* realized the accelerated topological

Table 2. A brief overview of design based on wave propagation characteristics in infinite meta-structures

Design type	Algorithm	Meta-structure and performance	Description	Year
Enhancing noise reduction	CNN		Predicted the absorption spectra of metasurfaces based on CNN and conducted experimental verification[106]	2021
	CNN CGAN		Prediction of sound absorption spectra of absorbers based on CNN and inverse design based on CGAN[107]	2022
	GAN		The generated structures can have completely new configurations and rich local features. They can be in good agreement with experimental results[108]	2021
	TNN		Overcoming the data inconsistency caused by the complex coupling effect between Fabry Perot channels, the experimental results are in good agreement[109]	2022
	RL		Exploring deep subwavelength broadband sound absorption meta-structures based on RL, replacing the artificial selection of structural parameters. The accuracy of the design was verified through sound absorption experiments[110]	2022
	RL		Employing RL to optimize the huge parameter space with nine aperture parameters to design broadband sound absorption meta-structures, and further validated through experimentation[111]	2023
	CNN		Inverse design of the absorber based on the target absorption spectrum by employing a one-dimensional CNN model. The difficulty lies in the selection of neural network structure and hyperparameters[112]	2021
	TNN		Inverse design of the absorber based on the target absorption spectrum by employing TNN. The model uses fewer hyperparameters and has higher accuracy and efficiency than traditional CNN[113]	2023
	MLP gaussian sampling		The inverse design incorporating probability sampling can obtain all possible structures. The transmission spectrum measured in the experiment is highly consistent with the predicted results, and the accuracy of the report is better than models such as ANN and GAN[114]	2020

	CGAN		Applying CGAN to generate sound insulation structure. The generated structure may not fully conform to physical laws, and the dataset may have a few duplicate samples[115]	2021
Advanced control of wave propagation characteristics	TNN		TNN effectively handles the increase in non-inconsistency of the dataset caused by non-local coupling effects[116]	2021
	TNN gaussian sampling		Introducing probability sampling in the middle layer of TNN, the design parameters have high flexibility, diversity, and robustness[117]	2022
	TNN gaussian sampling		A probabilistic model is a powerful tool to solve data inconsistency and has strong robustness to sensitive parameter design[118]	2021
	CNN GA		Employing CNN to achieve inverse design of metasurfaces based on multi-point sound pressure and the accuracy report is better than GA[119]	2021
	MLP		Replace the physical unit with MLP and transfer the input response, material properties, and output response of the whole system through the connection between MLPs[104]	2021
	MLP		MLP captures the relationship between the input and output wave responses of physical units to construct the overall structure and replace the time-consuming numerical simulation process[120]	2022
Optimizing topological states	Clustering		Through clustering algorithms, topological classification is carried out according to the real characteristics of the system, without prior knowledge and calculation of topological invariant[121]	2020
	MLP		Inverse design of phononic plate with anticipated bandgap width and topological property Using MLP. The quality of the edge state can be freely controlled through the preset bandgap width[122]	2021
	TNN		TNN overcomes data inconsistency and supports inverse design structures based on topological properties to achieve custom interface states[105]	2022

TNN		Experimental verification of the accuracy of using TNN to inverse design interface states[123]	2022
MLP GA		Efficient implementation of edge state design for specific or maximum bandwidth corresponding structures[124]	2022

design of metaporous materials with broadband sound absorption performance by GAN[108]. Liu *et al.* used cascaded inverse and forwarded CNN to achieve the inverse design of acoustic absorbing devices with coiled Fabry-Perot channels, which is based on the same principle as a fully connected TNN architecture[109]. Jin *et al.* used RL to optimize a lightweight sound absorption multi-function integrated meta-structure with perforated fish-belly panels[110]. Subsequently, they used this method to optimize a spiral plate sandwich structure that integrates lightweight, vibration reduction, and sound absorption functions[111]. Mahesh *et al.* proposed a one-dimensional CNN inverse design scheme for low-frequency Helmholtz resonate sound absorber[112]. Afterward, they further constructed a TNN architecture using inverse and forward one-dimensional CNNs for inverse design of a similar sound-absorbing structure[113].

Sound insulation is another method of controlling noise, with the objective of blocking or attenuating the transmission of acoustic waves. It typically relies on the transmission coefficient to characterize the performance of the sound insulation structure in blocking sound energy. For the design enabled by ML in sound insulation meta-structures, Luo *et al.* provided a paradigm of fuzzy design to overcome the problem of data inconsistency, as shown in Figure 3A[114]. Specifically, they combine MLP with mixed Gaussian sampling, mapping a target transmission spectrum to multiple sets of Gaussian sampling parameters through MLP and then linearly overlaying these Gaussian distributions to obtain a mixed Gaussian distribution. All acoustic meta-structures corresponding to the local maximum values are alternative structures that meet the target transmission frequency spectrum. Gurbuz *et al.* used a random algorithm to generate binary images of units composed of fluid elements and solid elements and obtained the transmission loss spectra through the finite element method[115]. Then, by training CGAN to capture the potential relationship between transmission loss spectrum and unit geometry, they carried out inverse design of the structural units to achieve the required sound insulation purpose.

Advanced control of wave propagation characteristics

Subwavelength scale metasurfaces may experience significant losses due to the presence of viscous friction and narrow acoustic channels. The diffraction acoustic meta-grating designed based on diffraction theory can improve the control efficiency of the acoustic metasurface. Ding *et al.* employed the TNN model to achieve inverse design of non-local metasurfaces for acoustic wave diffraction characteristics[116]. They explored the coupling effect between all subunits rather than nearest-neighbor coupling, demonstrating the ability of non-local metasurfaces to reshape the acoustic field. Meanwhile, the implementation of this work effectively demonstrates the ability of TNN to support the design of non-local coupled metasurfaces, especially in the face of complex coupling effects that greatly increase the degree of nonlinearity. In another work, Du *et al.* designed acoustic meta-grating wavelength division multiplexing by using an improved TNN architecture[117]. Specifically, they introduced probability sampling in the TNN architecture, which divides the design space into two layers instead of the traditional one layer for design parameters. Among them, the latter layer is the design parameters of the structure, obtained by sampling from the Gaussian

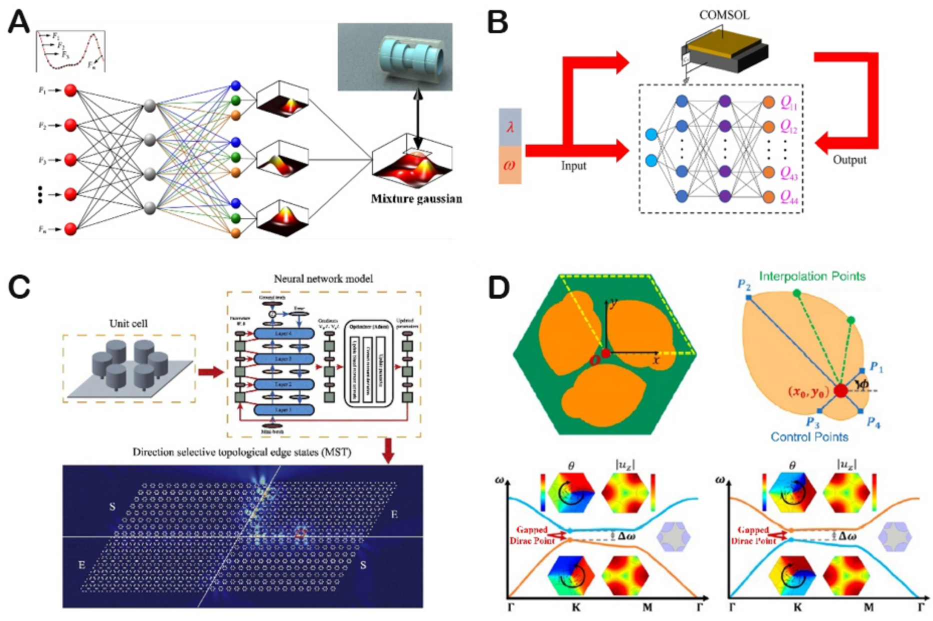


Figure 3. ML for the design of wave propagation characteristics in finite meta-structures. (A) Fuzzy design of acoustic meta-structures by combining MLP with Gaussian mixture sampling[114]. (B) Employ MLP to realize global transfer matrix prediction of active metabeams[120]. Reproduced with the permission of Ref.[120] Copyright 2020, Elsevier. (C) Employ MLP to realize the design of metaplates with robust edge states[122]. (D) Design of Valley Hall acoustic topological insulator by combining MLP and GA[124].

distribution parameters of the previous layer. The probabilistic TNN model has a strong generalization ability, greatly reducing the design cost of acoustic meta-grating wavelength division multiplexing. It demonstrates the flexibility, diversity, and robustness of design parameters.

The acoustic cloak technology aims to reduce the sound signals generated by objects in order to reduce the detectability of the sound detection system and achieve the effect of stealth. Ahmed *et al.* implemented a design of a multilayer core-shell acoustic cloak using probabilistic TNN architecture, demonstrating its effectiveness in solving the problem of high sensitivity of stealth cloaks to design parameters[118]. Stealth requirements weaken or even eliminate the disturbance of objects to the sound field, while in some practical needs, it is desired to freely weaken or enhance the sound field in certain specific areas. In this aspect, Zhao *et al.* proposed a CNN-based inverse design of metasurface phase gradient to achieve the regional control of sound field enhancement or attenuation[119].

In addition, research has attempted to enable MLP to learn the physical mechanisms of a single unit and then use it to construct a functional analysis of wave propagation in the overall structure. For example, Wu *et al.* used MLP to learn the input-output relationship of longitudinal waves in non-uniform thin rod elements and then assembled multiple MLP elements to construct a non-uniform overall structure[104]. A series of cascaded MLP units describe the input-output relationship of the overall structure and then use optimization algorithms to determine the design parameters of each individual unit. Similarly, Chen *et al.* used MLP for transfer matrix prediction of active metabeam elements, as shown in Figure 3B[120]. In their work, the metabeam unit is constructed by affixing a piezoelectric material on the main beam and connecting a negative capacitance circuit. By using COMSOL software to obtain transfer matrices for different capacitance values and frequencies, a dataset is constructed and used for MLP training. The global transfer matrix of the array elements can be obtained by connecting multiple groups of MLP in sequence, then the output and input signals of the whole metabeam can be connected.

Optimizing topological states

A topological state is also an important form of wave characteristics in finite structures. We now turn to focus on some recent design works on topological states. Generally speaking, topological invariants can characterize topological properties of structures, but their definition and calculation are often difficult. In essence, topological properties certainly exist in structural features, so exploring topological properties from actual structures instead of relying on topological invariants is another idea for topological classification. Long *et al.* demonstrated an unsupervised clustering algorithm for extracting topological features of phononic crystals, thereby classifying topological properties[121]. He *et al.* achieved the inverse design of phononic crystal thin plates with anticipated bandgap width and topological property based on MLP, as shown in Figure 3C[122]. By designing two units with a broadband common bandgap, they constructed a highly robust localized edge state for bending wave transmission. This group subsequently proposed using TNN to achieve the inverse design of phononic beams from topological properties to structure[105]. The topological properties of the bandgap were characterized by the reflection phase, and the interface states of one-dimensional phononic beams were predicted and constructed using TNN. Afterward, Muhammad *et al.* also completed a similar work[123]. Du *et al.* realized the inverse design of Valley Hall acoustic topological insulator by combining MLP and GA, as shown in Figure 3D[124]. Specifically, they first trained regression neural networks and classification neural networks for predicting bandgap and topological properties, respectively. Then, two neural networks are put into the optimization process of GA to obtain two structures with opposite topological properties under a common bandgap for constructing edge states.

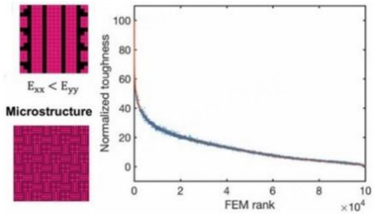
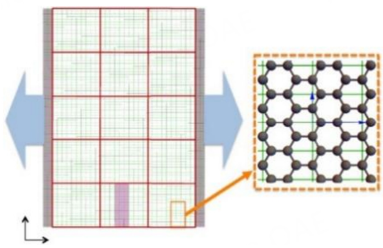
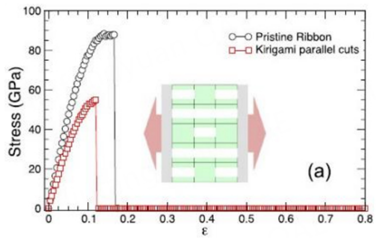
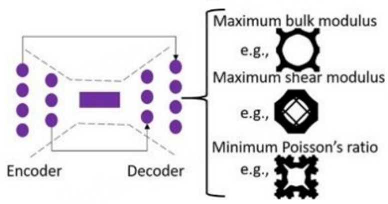
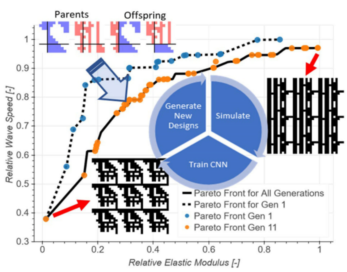
The application of ML in Hermitian systems mentioned above is still in the initial stage, and more achievements need to be further expanded. At the same time, we have also found that ML has recently made some attempts in non-Hermitian systems. Yu *et al.* used diffusion maps to unsupervised manifold learning of topological phases in non-Hermitian systems[125]. Different from the unsupervised method, there are also some works that demonstrate training ANNs for supervised prediction of non-Hermite topological invariants[126-128]. The essential difference between unsupervised and supervised is that the former does not need labels and directly extracts topological invariant from the on-site elements of the model, while the latter relies on the calculated topological invariant as labels to construct data sets. In non-Hermitian systems, an exception point (EP) is an important feature that represents the critical point at which the system transitions from a real eigen-spectrum to a complex eigen-spectrum[129]. In the latest work, Reja *et al.* introduced neural networks for the characterization of EP[130]. They proposed a method called summed phase rigidity (SPR) to characterize the order of EPs in different models. Then, they trained MLP models to realize the prediction of EPs for two-site and four-site gain and loss models.

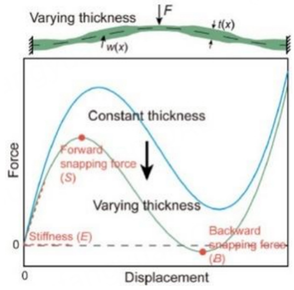
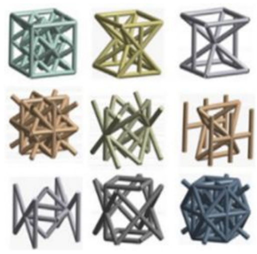
Design of static characteristics in mechanical meta-structures

Mechanical meta-structures have become an emerging growth point in the field of ML-enabling design due to their extreme statics performance. Combined with ML, meta-structures with excellent mechanical properties can be obtained through design optimization by adding, deleting, or changing. Table 3 provides a brief overview of ML for the design of static characteristics in mechanical meta-structures.

A lot of work has been carried out around the 2D mechanical meta-structures. These structures are usually designed and optimized on a plane to obtain specific shapes or material compositions with specific mechanical properties. CNN, as a high-quality model for image feature extraction, is widely used in the design of 2D mechanical meta-structures. Gu *et al.* proposed a self-learning CNN model to search for high-performance hierarchical mechanical structures[131]. This model can continuously learn patterns from high-performance structures, ultimately achieving design results superior to the training set. Hanakata *et al.* reported a design study on stretchable graphene kirigami, as shown in Figure 4A[132]. The cutting density and

Table 3. A brief overview of design based on static characteristics in mechanical meta-structures

Design Type	Algorithm	Meta-structure and Performance	Description	Year
2D structure	CNN		The inverse design of high toughness hierarchical structures based on CNN greatly saves computational time compared to traditional finite element methods[131].	2018
	CNN		Effectively searching for the optimal cutting mode for stretchable graphene kirigami structures under given yield strain and stress conditions based on CNN models[132].	2018
	Supervised AE		Generate the structure by passing potential variables to the decoder. It is expected to find new structures, but the prediction of mechanics performance beyond the dataset may be biased[133].	2020
	CNN		CNN for predicting 2D metamaterials with the best mechanical properties. The model exhibits robustness in terms of accuracy and inference time[134].	2020
	DCGAN CNN		Combine DCGAN and CNN for designing microstructures. The model has high efficiency and can flexibly control geometric constraints[135].	2019
	CNN GA		Combining CNN and GA can find Pareto's optimal structural design using a relatively small dataset, even with complex nonlinear constraints[136].	2021
	CNN GAN		Inverse design of 2D metamaterial based on predefined Poisson's ratio. The model can generate structures beyond the dataset and exhibit responses similar to real structures[137].	2022

1D/3D structure	MLP		Realize accurate prediction of variable thickness curved beams and their properties. Efficient and accurate optimization design results were obtained with different optimization objectives[138].	2020
	GAN		Generate lightweight and high load-bearing performance lattice structures using GAN and conduct experimental verification[139].	2021

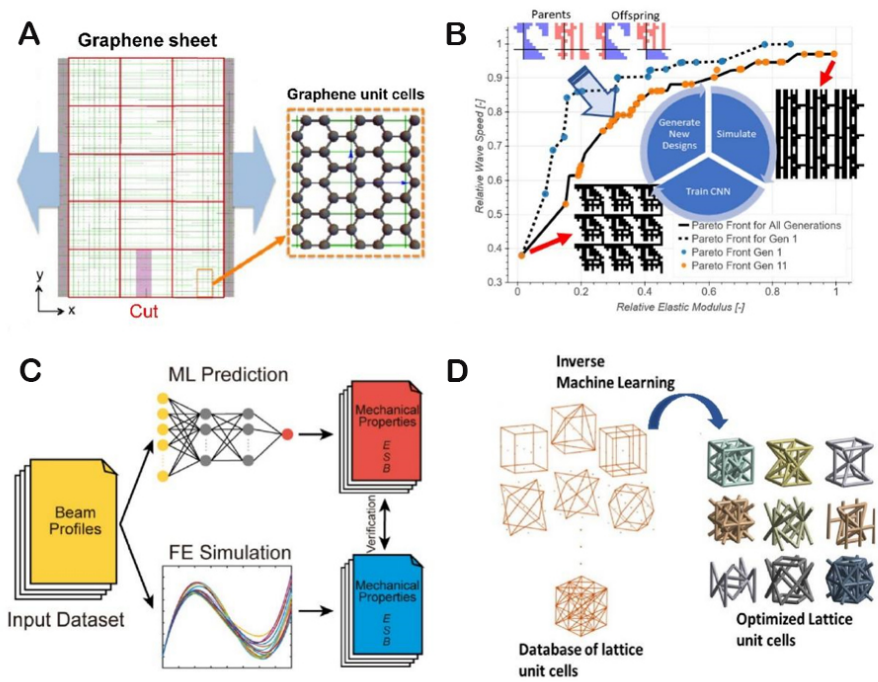


Figure 4. ML for the design of static characteristics in mechanical meta-structures. (A) Searching for the graphene kirigami with the best stretching performance through gradual training of CNN[132]. Reproduced with the permission of Ref.[132] Copyright 2018, the American Physical Society. (B) Combining CNN and GA to realize lattice metamaterial design satisfying additive manufacturing constraints[136]. (C) Design of curved beams with best mechanical properties based on MLP and optimization methods[138]. Reproduced with the permission of Ref.[138] Copyright 2020, Elsevier. (D) Design of lightweight lattice structures by GAN-based inverse design framework[139].

cutting position control the elastic stretchability of graphene kirigami. They first trained CNN through supervision to predict the stretchability of graphene kirigami expressed by yield strain. Then, in the inverse design, the CNN is trained using the dataset obtained from molecular dynamics calculations, and the model is gradually trained using the best performance predicted by the CNN. In subsequent research[133], they proposed a supervised AE to design graphene kirigami. Kollmann *et al.* reported the 2D metamaterial design with either maximum bulk modulus, maximum shear modulus, or minimum Poisson's ratio using CNN[134]. The dataset of their work is generated by the topology optimization framework based on the energy homogenization method and periodic boundary conditions.

To optimize the structure to obtain a 2D structure with the best mechanical properties, CNN is often combined with GAN or GA. Tan *et al.* reported a model in which deep convolutional GANs (DCGAN) are used to generate candidates adhering to geometric constraints, while CNN associates microstructures with properties[135]. After training, combine the two models for inverse design microstructural materials with specific mechanical properties. Garland *et al.* demonstrated the design of structural lattice metamaterial combining CNN and GA to meet the constraints of additive manufacturing, as shown in Figure 4B[136]. In addition, Wang *et al.* and Chang *et al.* also used this design paradigm to realize the inverse design of shell-based mechanical metamaterial and auxetic metamaterial with zero Poisson's ratio, respectively[140,141]. Tian *et al.* proposed the combination of CNN and GAN to achieve customized Poisson's ratio meta-structure design[137]. CNN is trained to predict the global Poisson's ratio response of a given meta-structure, while GAN realizes the structural inverse design of the anticipated Poisson's ratio response through adversarial training.

In addition, some works have been done to design and optimize specific mechanical properties of one-dimensional or three-dimensional (3D) meta-structures. Liu *et al.* demonstrated a design work of curved beams based on MLP and optimization methods, as shown in Figure 4C[138]. The mechanical properties of curved beams are characterized by stiffness, forward snapping force, and backward snapping force and are controlled by thickness distributions. They first trained MLP to predict the mechanical properties of curved beams with variable thickness and then put the trained MLP model into the optimization cycle proposed by Gu *et al.*, as mentioned above, to optimize the thickness distribution with the best mechanical properties[131]. Challapalli *et al.* demonstrated the GAN-based inverse design framework for optimizing lightweight lattice structures, as shown in Figure 4D[139]. The basic idea of this framework is to add initial conditions, boundary conditions, and forward regression to the real data distinguished by discriminators to obtain structural units with excellent performance. The new dataset is then used for GAN training, and the process is iterated repeatedly to obtain the structure with the best mechanical performance.

CONCLUSION AND OUTLOOK

In this review, we have discussed the combination and synchronous development of ML and meta-structure and reviewed the recent flexible applications of ML algorithms in the fields of acoustics, elastic, and mechanical meta-structures from the aspects of band structures, wave propagation characteristics, and static characteristics. Through analysis, we have come to the following main conclusions:

(1) The forward performance prediction of meta-structures can usually rely on analytical formulas or simulation software. The purpose of introducing ML is to save time and computing resources or to provide a forward computing part for some combined inverse design schemes. The inverse design of meta-structures is difficult to deal with analytically. DNNs with strong nonlinear modeling capabilities effectively solve this problem and can directly serve as alternative models for inverse problems. In addition, RL can also serve as an inverse design algorithm in meta-structures to explore structures that meet customized performance goals in the parameter space.

(2) A crucial issue in the inverse design process is how to alleviate data inconsistency. There are two main ideas. One approach is based on deterministic strategies, with representative approaches being: 1. TNN architecture with inverse and forward network concatenation. 2. Combining MLP (or CNN) with an AE.

The former achieves mapping from performance to features, while the latter achieves structure reconstruction from features. 3. Combining MLP (or CNN) with GA. The former achieves performance prediction through pre-training and then adds it to the iterative process of the latter. Another approach is based on probabilistic strategies; the main approach is to use Gaussian sampling after the data passes through the neural network rather than directly mapping to the structure or introducing Gaussian sampling in the middle design layer of the TNN architecture. Compared to deterministic strategies, probabilistic strategies have more diverse design choices.

(3) As the functional requirements of meta-structures become more critical, the design of meta-structures based on specific goals becomes more and more complex, which makes many advanced algorithms constantly develop and combine to meet the requirements. The support of an open-source framework makes the development of relevant algorithms for meta-structure design easier, even for the researchers without professional backgrounds in ML, which is an important reason for this field in a period of vigorous development and growth.

Although the research on the combination of ML and meta-structures has aroused great interest and attention in recent years, and many research achievements have been made, there are still many problems that restrict further development. The main problems and future directions can be summarized as follows:

(1) Obtaining data is often difficult, especially for problems without analytical solutions or high numerical calculation costs. Therefore, it is necessary to develop algorithms that only need small dataset training, such as reducing the demand for source data by transfer learning. Additionally, there is currently a lack of commonly used datasets in the field of meta-structure design. If researchers can share some datasets of conventional meta-structures, it will be easy to achieve data migration and fusion in the future.

(2) ANNs are often seen as black boxes, wherein the input of a set of structural parameters naturally results in the output of a corresponding set of performance parameters. Exploring what changes the data has undergone in the process of layer-by-layer transmission, in other words, how the structural parameters change step by step toward the performance parameters after each layer of operation, is important research to uncover the interpretability application of neural networks in the field of meta-structures.

(3) The research on some new physical concepts, such as non-Hermite smart phononic crystals, is in full swing in the field of meta-structures. What role ML can play in these new physical mechanisms is a question that can be deeply explored at present.

(4) The research of meta-structure mainly involves design and manufacturing. ML can theoretically provide excellent design results for various acoustic or mechanical requirements of targets, but most current research lacks manufacturing and experimental verification after design. Therefore, more consideration of manufacturing and verification is an important prerequisite for the application of this field.

(5) Multifunctional integration is an important direction of the development of meta-structures at present, which may involve the coupling of multiple physical fields, such as acoustics, mechanics, electromagnetism, and heat. Developing ML algorithms for multifunctional meta-structure design with multi-physical field characteristics is not only a challenge but also a promising direction. The path planning problem of multifunctional integrated composite meta-structure configuration in 3D printing containing continuous fibers is one of the important reasons currently restricting the manufacturing of complex composite structures. By introducing ML algorithms to optimize the fiber distribution direction field of continuous

fiber path planning, a collaborative optimization scheme between continuous fiber path and functional structure configuration can be achieved, which is expected to become an important means for the manufacturing of complex composite meta-structures in the future.

DECLARATIONS

Authors' contributions

Supervision, conceptualization, validation, project administration, funding acquisition: Jin Y, Li Y, Zhuang X

Original draft preparation, reviewing, and editing: He L, Li Y, Torrent D, Zhuang X, Rabczuk T, Jin Y

Availability of data and materials

Not applicable.

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Conflicts of interest

All authors declared that there are no conflicts of interest.

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Not applicable.

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