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Machine Learning and Deep Learning in Phononic Crystals and Metamaterials – A Review

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Abstract

Machine learning (ML), as a component of artificial intelligence, encourages structural design exploration which leads to new technological advancements. By developing and generating data-driven methodologies that supplement conventional physics and formula-based approaches, deep learning (DL), a subset of machine learning offers an efficient way to understand and harness artificial materials and structures. Recently, acoustic and mechanics communities have observed a surge of research interest in implementing machine learning and deep learning methods in the design and optimization of artificial materials. In this review we evaluate the recent developments and present a state-of-the-art literature survey in machine learning and deep learning based phononic crystals and metamaterial designs by giving historical context, discussing network architectures and working principles. We also explain the application of these network architectures adopted for design and optimization of artificial structures. Since this multidisciplinary research field is evolving, a summary of the future prospects is also covered. This review article serves to update the acoustics, mechanics, physics, material science and deep learning communities about the recent developments in this newly emerging research direction.

Keywords: acoustic metamaterial, deep learning, machine learning, mechanical metamaterials, phononic crystal

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1. General Introduction

Phononic crystals (PnCs) and metamaterials have emerged as the potential candidates for acoustic and elastic wave manipulation due to their structure-dependent peculiar wave dispersion and dynamic characteristics that are unattainable from natural materials. These fantastic wave phenomena are observed in the frequency bandgap (BG) regions where wave propagation is restricted. The frequency of propagating waves lying inside such BG cannot propagate through these periodic or aperiodic synthetic structures. Thus, it provides a favourable platform to manipulate the incident waves. The frequency BG property also enables different types of wave manipulation for metamaterial devices such as waveguiding, wave focusing, wave collimation, wave multiplexer, wave diffraction, wave absorption and attenuation, etc [1]. These intriguing physical phenomena and unusual dynamic characteristics offered by PnCs and metamaterials make them a prominent and viable solution for resolving multiple vibration and noise related engineering problems. Today research in metamaterials is both intensive and extensive in different engineering disciplines and communities. This research realm is gaining research momentum and it is now finding promising industrial and infrastructural applications in wave manipulation breakthroughs in vibration and noise control.

Before going into a detailed state-of-the-art review, a clarification on the main difference between PnCs and acoustic metamaterials (AMs) is necessary. Generally, these two terms are used in the literature interchangeably [1]. Although both terms belong to artificial structures that govern a frequency BG property, several differences are apparent. Briefly, a PnC is a periodic structure with elasticity modulus/density contrast that works on the principle of Bragg scattering physical phenomenon. Thus, BG is generated due to the structural periodicity and destructive nature of wave interference phenomena. Therefore, the opening of BG frequency is dependent on the periodicity characteristic constant and wavelength of propagating waves. Adversely, AM is a synthetic composite structure comprised of resonators that couple with the hosting media to generate subwavelength BG caused by wave hybridization [2]. Usually, the BG is induced at much lower frequencies, i.e., the so-called subwavelength scale, as compared to the Bragg scattering mechanism. In addition, these artificial composite structures can be periodic or aperiodic and due to the local resonance mechanism, the system periodicity shows limited effects on the opening and closing bounding edges of the BG [3, 4].

Thanks to wave hybridization effect, the opening of BG at subwavelength scale provides a promising avenue to manipulate waves of very low frequency at subwavelength scale with a much smaller unit cell structure. Due to this property, AMs are considered as a homogeneous material/continuum with effective medium properties, which induce many surprising physical phenomena under specific conditions [5-11] that have been considered non-natural using natural materials such as negative Poisson's ratio, negative stiffness, negative refractive index, for instances. Due to the Bragg scattering effect and system periodicity, PnC is not recommended for low frequency wave manipulation as very large size unit-cell structures are required.

Conversely, AMs are considered a prominent candidate for subwavelength wave manipulation due to their local resonance mechanism/wave hybridization, effective medium properties, and small size resonators. An extensive amount of theoretical research has explored the peculiar dynamic properties of PnCs and AMs for wave manipulation [12-14]. The reported works demonstrated the effective medium characteristics of metamaterials, including negative effective mass density [15], negative stiffness [16], double negative effective media [17], negative Poisson's ratio which are the so-called auxetic metamaterials [18], etc. The concept of auxetic structures has also contributed to the development of mechanical metamaterials/architected materials with unusual quasi-static properties. These peculiar properties have been also applied for subwavelength wave manipulation including subwavelength vibration and noise control [19], subwavelength acoustic and elastic waveguides [20], subwavelength focusing and lensing effects [21], acoustic rainbow trapping [22], subwavelength wave diffraction [23], acoustic and elastic cloaks for making an object invisible from incoming waves [24], Umklapp effect [25], photo-resistive effect [26], flat-lens effect [27], acoustic meta-equalizer [28], nonreciprocity phenomena in acoustic and elastic materials [29], inertially amplified resonators [30], topological insulators with protected interface states [31] etc., in acoustic and elastic systems.

Mechanical metamaterial, or architected material, is another emerging research topic that has gained increasing research interest due to its novel design principles derived from hierarchical architecture and biological animals with material size effects at a micro/nanoscale [32]. This metamaterial-based design method is shown to have better mechanical performance that enables us to colonize hitherto uncharted territory in the material property space, such as areas with extremely high strength-to-density ratios, exceptional resilience, and energy-absorbing properties with brittle components. This branch of metamaterial should not be mixed with PnCs and acoustic/elastic metamaterials, which are mainly studied for wave manipulation and propagation. Rather, this type of artificial materials are more focused on quasi-static properties with tunable stiffness, auxetic behaviour, negative compressibility, vanishing shear modulus, etc.[16]. Recently, a new class of responsive materials are also proposed with tunable, reconfigurable and programmable mechanical properties in both space and time [32].

Thanks to advancements in additive manufacturing technology that allow fabrication of such architected designs with complex architectures across multiple length scales, with characteristic sizes down to nanometer scale for a wide range of materials [33, 34]. Due to the *size effect*, for some architected designs significant strength gain compared to bulk counterpart is observed and it led to a trend that *smaller is stronger* in materials [35, 36]. A detailed discussion about mechanical metamaterials is outside the scope of this review and interested readers may refer to further references [32, 37, 38]. Since machine learning (ML) and deep learning (DL) methods have seen surge of research studies for inverse design and optimization of architected designs, we are limited to a brief overview on this particular aspect of this topic. In a nutshell, today the notion of metamaterials is not limited to theoretical concepts and physical phenomena. The potential application of metamaterial has been explored for noise insulation [39], low frequency vibration control [3, 40], aeroacoustics [41-43], soft robotics [44, 45], automobile applications [46, 47], earthquake applications [48], underwater acoustics [20, 49], low-pass mechanical filters [50], energy harvesters [51], smart materials [18, 52, 53], MEMS and NEMS technologies [54, 55], nature-inspired metamaterials [56, 57], bio-medical applications [58], etc.

2. An Overview on Optimization Methods

Optimization techniques have a crucial role in optimizing structural designs and improving metamaterial performance. This is because metamaterials are man-made engineered structures with effective medium properties, dynamic and quasi-static characteristics and peculiar wave dispersion that are dependent on the designs of unit-cell structures. Despite the multiple underlying principles, governing mechanisms, structural configuration, material properties and so forth, traditionally the design of PnCs and AMs depend upon physics-inspired methods. The design process is guided by human knowledge, such as physical insights gained through studying basic systems, experience gained from past practices, and intuitive reasoning. Initial designs are often tested using simulations that solve the governing partial differential equations, although sometimes experimental results are less likely to directly match the intended performance. A primary cause for this discrepancy can be the difficulty in achieving the required manufacturing tolerances in complex geometries reliant on additive manufacturing [59-61]. To approach the design objective, changes to a handful of parameters and re-evaluation by simulations must be repeated on an iterative basis. While this method has had a lot of successes, the trial-and-error method is becoming increasingly computation-expensive and time-consuming as the complexity of AM design grows. On the other hand, inverse design methods tackle this task in a different manner. Without the use of physical principles for the initial guess, the intended acoustic functionalities are obtained through optimization in the design parameter space, which seeks a solution that minimizes (or maximizes) an objective/ fitness function related to the target using advanced algorithms and combined simulations. Likewise, in relation to solving the direct problems, optimization-based approaches require comparable computation time and power. However, they enable one to search the entire parameter space for designs that are non-intuitive but perform well.

Whether we discuss the individual unit cell or array of metamaterials, structural design plays a vital role in defining the peculiar dynamic properties and wave dispersion. To date there are two design approaches that are commonly applied. First, the physics based methods including simplified analytical models with prior or relevant practical knowledge and scientific insights. A good example is Mie theory [62] that allows quick and accurate modelling of simple geometries such as cylinders, spheres and core-shell elements to design three-dimensional PnCs with desirable absorptive properties. In PnCs research the Mie scattering theory has been widely studied to manipulate phonon transport. Likewise, in AM researches the mass-spring analytical model is largely utilized to investigate the peculiar dynamic properties and design efficient structures for vibration control [40, 63, 64]. Although these analytical models and physics-based design provide useful guidelines to find the suitable physical parameter, structural configuration/ topology, realizing desirable performance is not an easy task, especially when the structure shape and spatial arrangement (both in term of topology and material distribution) are complex. Therefore, we have to depend upon the second approach that is based on numerical simulations, commonly by finite element method, finite volume method, boundary element method etc., with or without optimization algorithms. In general, these computational methods solve the PnC and metamaterial design issues by discretizing the partial differential equations of wave motion spatially and temporally, beginning from specified initial boundary conditions. The dynamic properties of representative unit-cell structures can be accurately calculated by defining sufficient meshes and iteration steps. In this process, often we need to fine tune the geometric properties and perform simulations iteratively to gradually come closer to the desired results. Now this process largely depends upon some prior experience with design templates owning to constraints like computational capacity and simulation time. As a result only limited design parameters can be adjusted while searching for an optimal performance. This is quite tedious, and it is computationally expensive with limited freedom in the design space.

The inverse design technique, defined as the direct retrieval of the proper structure for the specified dynamic performance, necessitate a significantly greater degree of flexibility in the design space, thus making it much more complicated and challenging. Now this design procedure is usually guided by optimization algorithms to efficiently search the latent space either via gradient free methods including evolutionary approaches (for example genetic algorithm (GA) [65, 66]) or gradient based methods that include topology optimization (TO) [67-69], and level set method or adjoint methods. In many cases, PnC and AM structures can now be discovered using inverse design algorithms that surpass structures created by empirical studies. Basically, these algorithms are rule-based techniques that include iterative searching processes in a case-by-case manner, typically depending on numerical simulations to generate interim findings that contribute to the modification of the searching strategy. Due to the random search nature, such stochastic algorithms are insufficient for sophisticated design in a multi-constrained problem. Interested readers may refer to references [70-72] for reviews on the inverse designs in photonic and phononic systems.

On the other hand, artificial intelligence (AI) based ML and DL methods have transformed several fields of science and engineering including materials science [73], chemistry [74], particle physics [75], computational mechanics [76], quantum mechanics [77] due to its exceptional success in domains related to computer science and engineering, such as computer vision [78], speech recognition [79], knowledge graphs [80], and decision making [81], demonstrating their potential to overcome the limitations of a bottom-up, physics based design strategy. A brief history is discussed in the next section. ML is a branch of AI and DL is one part of the ML with deep neural networks. Over the recent past these data-driven methods have emerged as a revolutionary new technique to model and design artificial materials. Of course, some limitations exist and they are briefly explained in Section 6 of this review. The distinct benefits of ML and DL stem from the data-driven approach, which, in contrast to physics- or rule-based approaches, enables the model to automatically uncover and map meaningful information from a large quantity of generated data. The data-driven feed-forward and back propagation design strategy are another attribute of this approach that make it attractive for design optimization of artificial structures.

Artificial neural networks (NNs), which were basically inspired by biological neural networks, have revolutionized data processing by enabling the development of algorithms that can "*learn*" from data and execute functions to complete complicated tasks [82]. Therefore, ML and DL and their related techniques are seen as a viable contender for inverse design of new artificial materials including PnCs [83], AMs [84] and nanophotonic devices [85]. In general, the role of DL in metamaterial is to explore design space to best match the target. However, unlike other optimization approaches like GA and TO that do this for every design sample, which makes the simulations recurrent and time demanding, the ML and DL algorithms are capable of navigating in a smart way by learning from a large dataset so that a design solution can be achieved quickly following the learning phase. Therefore, when an input database is provided for a set of applications, this data-driven method significantly reduces the total computation time without sacrificing design flexibility.

Because the wave dispersion and dynamic characteristics of metamaterials are dependent on physical design parameters like topology, the use of ML and DL methods are therefore interactive i.e., from physical design to frequency response spectra and vice-versa due to the forward and backward propagation learning processes, for more details see ***Appendix***. Because their integration is in its infancy, it will be relevant and helpful to provide an overview of this new subject. Hence, the interested readers can understand the fundamental concepts and solve the existing problems. Since there are multiple review articles that discussed the other optimization approaches like TO [68] and inverse design methods [85], there exists an essential need for an updated review that summarises the recent findings of ML and DL data-driven methods in the field of PnCs and metamaterials. Although a review article on intelligent nanophotonics [85] and photonic crystals [86-88] have been published earlier where the implication of ML and DL methods for nanophotonics and photonic crystals are discussed, this review article tends to focus on the recent advances in PnCs, AMs and architected materials by ML and DL methods.

The review begins by providing a brief overview of PnCs, AMs and mechanical metamaterials that outlines the need for optimization methods. We also discuss the history of DL model applied for photonic, phononics and mechanics research, as well as the conception, development and advantages of ML and DL networks. Afterwards, from the basic multilayer perceptron (MLP) to advanced deep neural networks (DNNs), we discuss several major model architectures, emphasizing their potential to design artificial materials/structures. These data-driven models can relate design attributes to metamaterial properties that allow for both forward and inverse designs. We also cover the state-of-the-art developments regarding DL methods in PnCs, AMs and architected materials/mechanical metamaterials. Finally, we discuss the prospects and limitations of this developing multidisciplinary research topic which has the potential to build a new scientific and engineering paradigm.

3. History

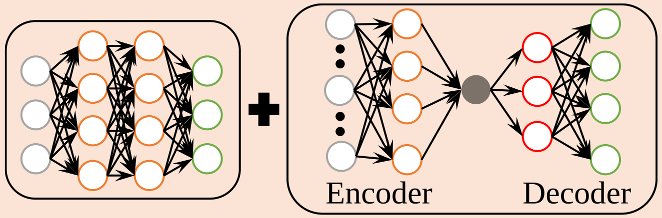
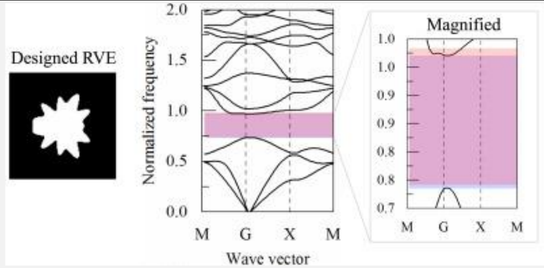
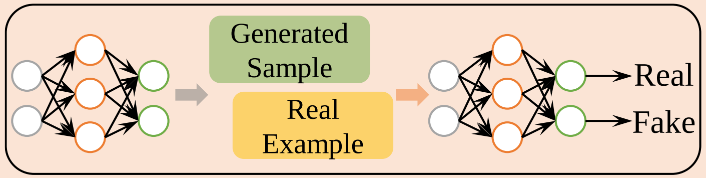
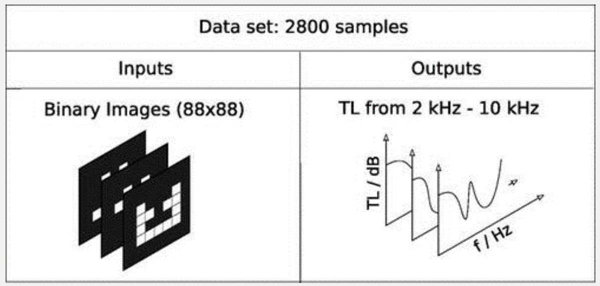
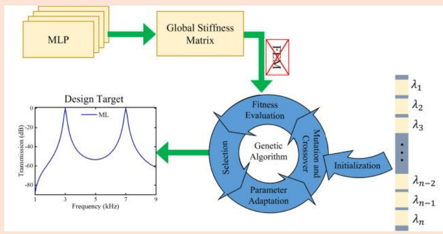
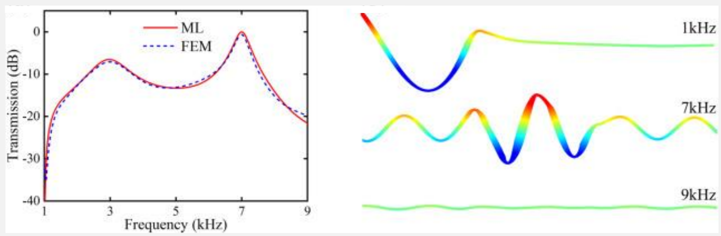
DL has a long history dating back to the 1940s, and it has gone by numerous names before being generally recognized as this term [89]. Fundamentally, some of these learning algorithms were created with the intention of computationally modelling biological learning – that is, how learning process occurs in human brains. As a result, since 1980s, DL has been referred to as artificial neural networks (ANNs), which coincided with the second wave of AI research, partly driven by a moment known as connectionism [90]. The famous paper written by David Rumelhart, Geoffrey Hinton, and Ronald Williams in 1986 [91], that modified and reiterated the significance of the original back-propagation algorithm, attempting to make it much efficient than prior approaches to learning and enabling it to solve previously unsolvable problems, was a watershed moment during this period. In 2006, Hinton, who subsequently coined the phrase "*deep learning*", demonstrated that DNN could be effectively taught using an approach termed greedy layer-wise pretraining [92]. DL grew in popularity when researchers were able to train deeper neural networks than had previously been feasible, and the theoretical significance of model architectural depth was discovered. Further, aided by the ever increasing size of the accessible data and computation power such as advanced GPUs, hardware supports, open source flexible software (PyTorch, TensorFlow and Keras, etc.), DL continues to dominate the AI research with network performance exceeding prior models by a significant margin, in fact defeating human brains in a number of cases [93].

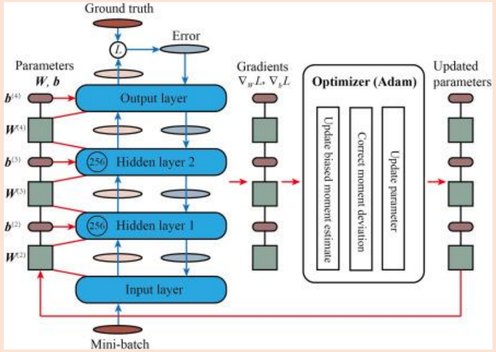
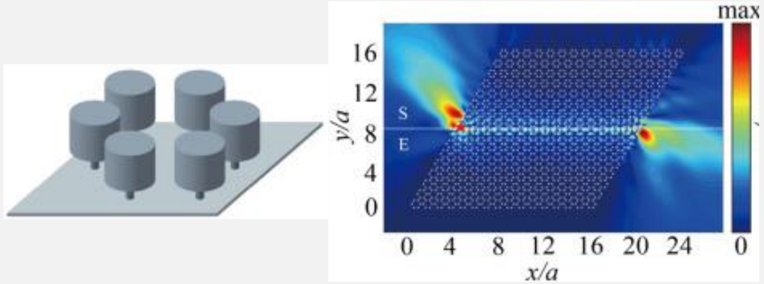
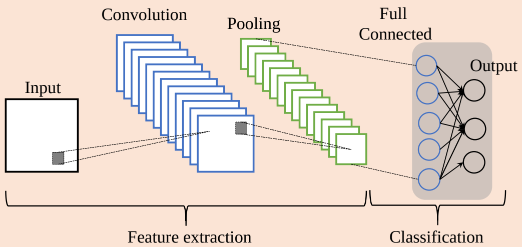
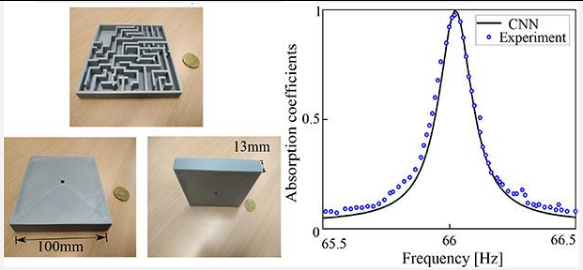
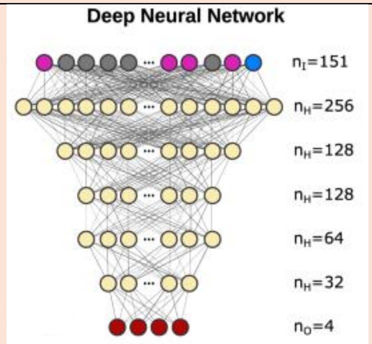
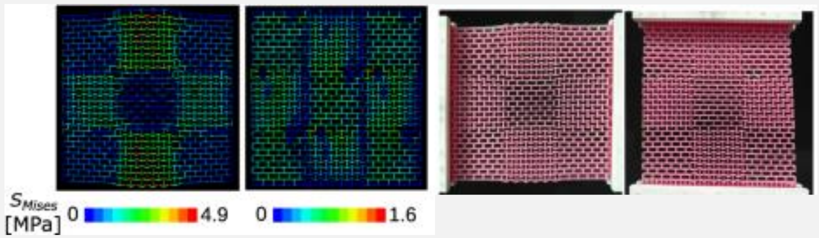
Since the idea of PnCs and AMs is fundamentally inspired by pioneering findings in photonic and electromagnetic counterparts, a brief context on the application of DL in later domain is informative. The introduction of DL (more appropriately ANNs) in photonic research can be dated back to early 1990s. In the microwave community, the ANNs were employed as a computer-aided design tool for quick prototyping of microwave devices and radio-frequency circuits [94]. The revival of the MLP (as simplest form of feedforward network consisting of multiple neuron layers) was attributed to the success of ANN-aided design. In this type of network, the neuron in each layer is connected to all other neurons in the preceding layer, see ***Appendix*** for more details. Therefore, sometimes it is also refereed as dense or fully connected neural network. The implementation of ANNs was not complicated at this early stage. The design optimization problem was usually translated into training an ANN that links the input layer to an output layer. Depending upon the nature of the task, usually microwave circuit or device parameters (e.g., physical property, geometry, frequency) or performance variables (e.g., voltage, current, power) were carefully selected to pass to the input layer of the network. Based on this framework, multiple types of microwaves design issues were solved [95]. Later, this data-driven strategy was widely adopted for the design, optimization and performance enhancement of other photonic dielectric structures [96-102] and devices [103].

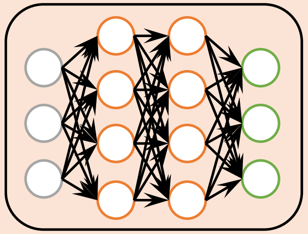
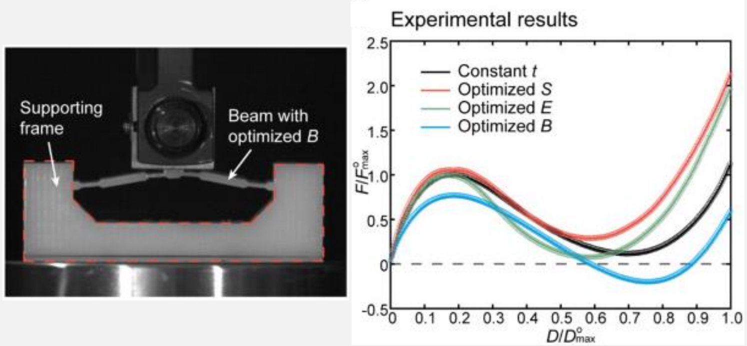
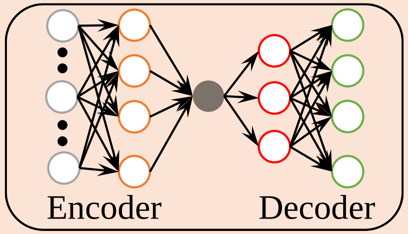
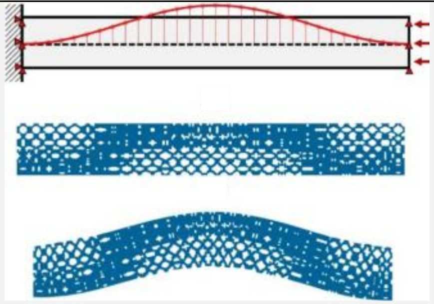
In almost all studies, the goal of the training process is to optimize the model parameters to make it more accurate based on input database. The training data maps the input variable X with potential output Y through a mechanized mapping. Beginning with random initialization, this data-driven algorithm learning strategy iteratively updates model parameters on the training dataset according to a predefined loss function assessed on the true output Y, until the generalized model so developed is able to predict unseen data. Compared to this approach, the conventional optimization strategies like GA, TO and other gradient based or gradient free methods which lack pre-defined input-output pairs and optimization is performed without any preconceived shape information in a case-by-case manner within a limited design space.

It was not a coincidence that photonic and phononic research and ANNs collied as the first attempt to merge wave propagation and manipulation with AI. Since the quasi-static and dynamic properties of metamaterial depend upon the structural design morphology rather than material parameters, optimizing a particular parameter for a given target is convenient by ML and DL methods. This method is so efficient that with some matured simulation tools, well-understood physics and little difficulty in data generation, a MLP model can develop a relationship between these parameters/variables to achieve a desirable output in a more computationally efficient manner. Again, this depends upon the type of problem. Furthermore, this research realm has observed a surge of studies with the invention of new training and regularization techniques such as rectified linear units (ReLU) activation function [104], batch normalization [105], dropout method [106] etc. This made it possible to develop and train deeper neural networks with the capability to exploit large datasets with better performance. Depending upon the problem types and desired output, various type of neural network architectures such as autoencoder (AE), convolutional neural networks (CNNs), generative adversarial network (GAN), recurrent neural network (RNN) and variational autoencoder (VAE) etc. have been developed for design optimization and performance enhancement of artificial materials. The description of network architecture and working principles are covered in the next section.

Table 1: Machine Learning and Deep Learning methods adopted for inverse design and optimization of phononic crystals and metamaterials.

Network Type	**Network Architecture**	**Metamaterial Design and Performance**	**Description**
MLP+CNN			Inverse design of phononic crystal with magnified bandgap [83]
GAN			Inverse design and optimization of acoustic metamaterials [84]
MLP+GA			Inverse design of multifunctional metabeam [107]

MLP			Inverse design of topological metaplates with topological interface mode [108]
CNN			Ultrathin acoustic absorbing metasurface [109]
MLP/DNN			Inverse design of 3D-printed mechanical metamaterials [110]

MLP			Inverse design and optimization of mechanical beam [111]
AE			Inverse microstructure design of metamaterial system [112]

4. Neural Network Architecture and Working Principle

This section will explain the basic network architectures. In the next section, we relate the state-of-the-art developments in PnCs, AMs and mechanical metamaterials that are relevant to these networks. A brief correlation is depicted in Table. 1. As described in the prior section, since early discovery of NNs in 1980s, the research domain has expanded and resulted in the discovery of numerous types of network architectures with distinct working principles that differentiate them from each other from the application point of view. Therefore, prior to applying these networks for PnC and metamaterial research, an understanding of network architecture, working principle and algorithm learning processes is necessary. Such insights will help the research community understand the network architectures and apply them appropriately to solve the existing challenges. These networks are distinct from each other in multiple aspects and they can be classified into three major categories: supervised learning, unsupervised learning, and reinforcement learning (RL). See ***Appendix*** for a detailed discussion about the working principle of fully connected NN and back-propagation algorithm.

4.1. Supervised learning networks

4.1.1 Multilayer Perceptron (MLP)

This is the most common type of ML network developed [113] and reminiscent of human brain architecture where data is collected, parsed and learned. As shown in Fig. 1, in this type of network many artificial neurons map the input data to the output by multiple layers of connections. Each neuron in the input layer is connected to all the neurons in the succeeding layer. Therefore, this type of network is also referred to as a fully connected neural network or MLP. Here, the training samples are comprised of input eigenvectors (x) and labels (y). For example, in cases of PnCs and AMs, the band structure is converted into binary eigenvectors where the passband and BG are represented with 1 and 0, respectively [83, 114]. This information is provided to the input layer with a set of pre-defined geometric parameters. By forward propagation the network is trained to establish a relationship between band structures and physical parameters. In this forward training process, the weights (w) of the network are set as constants. After training, in the backpropagation learning process, the weights are varied to correctly predict the band structure for a set of newly defined physical parameters, see ***Appendix*** for more details. The basic mechanism is to predict an unknown function f that relates $y=f\,(x;\,W)$, where W represents the neuron weights (w) and bias (b) between each layer that is determined and varies during the training process. The discrepancy between input training data and output predicted result is quantified by the cost function (C_σ). The objective of training phase is to use the gradient descent approach to minimize C_σ while updating (w) and (b) layer by layer.

The training process of the model is controlled by a set of hyperparameters. These hyperparameters are tuned to increase the efficiency of the network learning process and to reduce the computational cost. One of the parameters is the learning rate (α) which updates step of the weights in each iteration of the algorithm. This α of the classic gradient descent approach is quite sensitive, and this problem is especially prevalent in high-dimensional space and multilayer networks. Hence, if α is kept as a small value, the network learning process is slow and thus it takes more time and computation for learning. In contrast, if α is set as a very large value, the learning process is quicker however we may miss the extreme points. Also, if α is kept at a fixed value throughout network learning, it gets stuck at the saddle point during the iterative process. In order to solve this issue, it is important that α should not be a fixed value and it must be automatically adjusted within each iteration. To do so, usually an adaptive optimization algorithm like Adam, RMSProp, or AdGrad is applied.

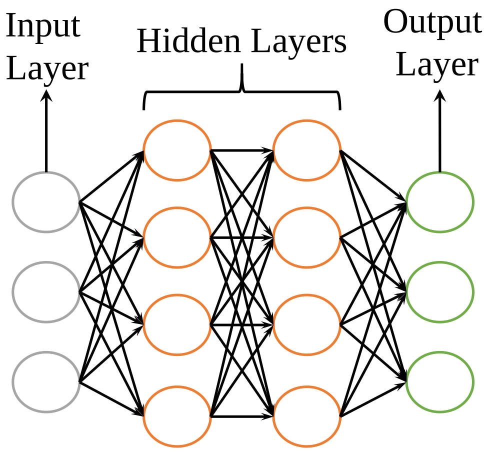


Fig. 1: Architecture of multilayer perceptron (MLP).

After the training process, some unseen test samples are used to validate the model accuracy. The trained and tested network can be applied for predictive modelling. Recently, this approach has been applied for the design of PnCs [83] and topological beam [114]. Generally, if the activation function is appropriately selected and the network has sufficient neurons, the network with one hidden layer can continuously map the function from input data to output counterpart. The capability of NN to capture the nonlinear qualities of a high-dimensional space makes it useful for capturing the complicated nonlinear correlation between structures and properties (or properties and structures).

4.1.2 Convolution Neural Network (CNN)

Furthermore, CNN is another type of ANN used for the design of artificial materials. The generated data is passed to an input layer that is connected to hidden layers also called convolution layers, polling layers, fully connected layers and normalization layers, see Fig. 2. Recently, Donda et al. [109] applied CNN to design an ultrathin acoustic absorbing metasurface for sound absorption. By applying the convolution process, the features are extracted from the input metasurface data and they are passed to a pooling layer for feature selection and filtration. By repeating this process, the output sample is obtained by a fully connected layer of neurons. Generally, CNN is useful in feature extraction from images that can efficiently map the field images to output response. Like in Donda et al. [109], the metasurface features are connected to a frequency absorption coefficient for inverse design, optimization and performance improvement.

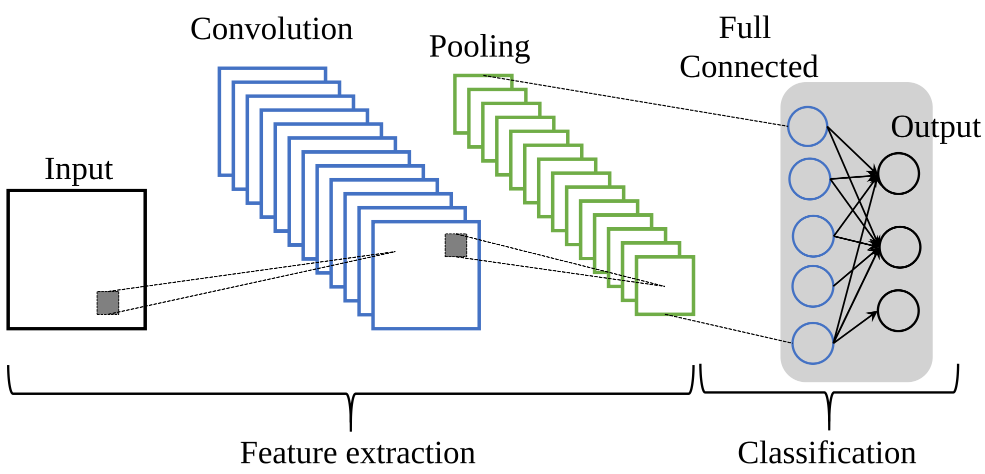


Fig. 2: Architecture of convolution neural network (CNN).

4.2. Unsupervised learning networks

Compared to the supervised learning network where training occurs based on labelled samples, the unsupervised learning analyses unlabel samples and try to find the mapping/structure or distribution law for the sample set. The two famous methods include clustering and data dimensionality reduction. Clustering divides the input data into different classes without training process. The fundamental challenge of clustering is to explore the ways on how to identify various classes because there is no explicitly specified category standard. As a result, several clustering methods have been developed based on various class definitions including probability distribution, centroid, and density. Through linear or nonlinear dimensionality reduction techniques like the principal component analysis (PCA) and manifold learning, higher-dimensional data can be translated to lower-dimensional space, thus making the analysis and classification easier.

4.2.1 Generative Adversarial Network (GAN)

GAN is an unsupervised learning network that has been widely used for various applications. Recently, material designers and engineers using PnCs and AMs have seen promising applications for efficient design optimization. This type of NN has two components, i.e., *generator network* and *discriminator network*, see Fig. 3 for details. They have their own functionalities and both networks do compete with each other to outsmart their rival. Interested readers are referred to a comprehensive tutorial [115]. Often created by MLP, the generator gets the random data as input and generates some new samples. The generated samples are taken as input data together with real samples (input of generator) and fed into the discriminator network. The discriminator works on the principle of binary classification. It distinguishes the real and fake samples (samples generated by generator network to outsmart the discriminator) and pass these results to update the model. Hence, to deceive the discriminator, the generator must learn the probability distribution of the real samples and make the generated samples similar to the real samples as much as possible. The job of discriminator network is to discriminate between real and fake samples with high precision. The performance of the two networks are optimized in parallel during the training phase and this process stops when the data classification accuracy of the discriminator reaches 0.5. This shows that the discriminator network can no longer distinguish between real and fake data samples and the model has achieved satisfactory balance. Sometimes the generator network cannot generate fake samples and the generated data is very similar to real samples. This problem is usually observed in the conventional GAN. To solve this problem, some recent studies have adopted conditional GAN to optimize the system performance [84]. Apart from generating new samples from real ones, this conditional GAN network also utilises some conditions based on characteristics of the real samples. Recently, Gurbuz et al. [84] applied conditional GAN to optimize the transmission loss of an AM array comprised of solid and fluid domains. The input samples and their sound transmission loss property are fed into the generator as input. The networks are trained and it is observed that the training process for the conventional and conditional GAN are same. After training, the network was able to predict the AM unit-cell structure for a target transmission loss frequency.

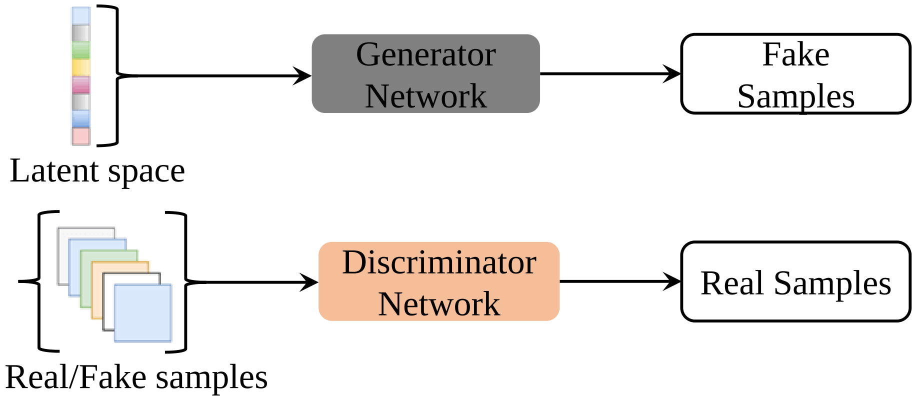


Fig. 3: Architecture of GAN with generative and discriminative networks.

4.2.2 Autoencoder (AE)

AEs are a type of DNN structure that uses the strong nonlinear processing capacity of NNs to extract features from the input data and for minimizing data dimensions. It consists of two parts referred to as the *encoder* and *decoder*, see Fig. 4 for more details. The task of the encoder is to extract features from input data. The decoder reconstructs the input samples based on the features available in the original input samples. After passing the input samples through the encoder and then decoder to produce the output vector, the reconstruction error is calculated by comparing the output vector to the original input vector. This reconstruction error is also referred to as the cost function and it can be minimized by applying the back propagation algorithm. In the perspective of PnC research, Li et al. [83] applied this approach to optimize the topology and magnify the width of BGs.

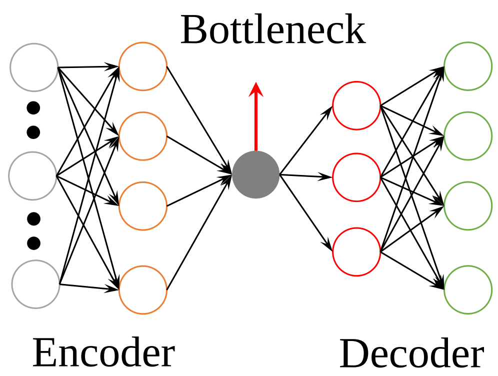


Fig. 4: Architecture of AE network.

4.2.3 Tandem Neural Network (TNN)

Inspired by the idea of AE, TNN has recently been applied for the design of artificial materials. Like GAN and AE, it also consists of two parts, i.e., inverse network connected with pre-trained forward network, see Fig 5. In this approach, first the forward network is designed as a pre-trained network by providing input data and getting the output response. This forward network works on the principle of supervised learning. Since each structure corresponds to a single response this is sometimes termed a one-to-one problem. While training the TNN, the weight and bias of the forward network is kept fixed and the cost function is reduced by adjusting the weight and bias of the inverse network. This can be done by using some adaptive optimization algorithms like Adam, RMSProp, AdGrad, etc. The difference between predicted response and target response define the cost function. In this type of network, the desirable response is kept as the input and potential design structures are obtained from the intermediate layer. In the network training process, the input response (output response of pre-trained network) are also used as labels, therefore this step is considered as an unsupervised training. In comparison to AE, the training of TNN is more cumbersome but it can correlate the structure with response without feature extraction. In fact, if one wishes to train input images, the AE or TNN can be replaced with a CNN without changing the fundamental principles. A good example of TNN has recently been reported by He et al. [114] for analysing and designing a topological phononic beam.

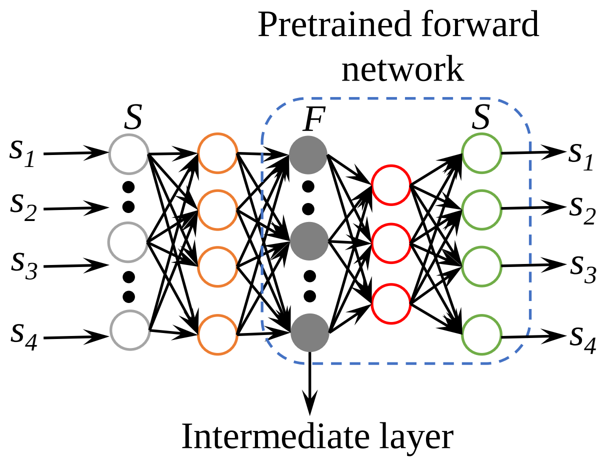


Fig. 5: Architecture of tandem neural network.

4.3. Reinforcement learning networks

This NN is fundamentally inspired by behaviourism and it works based on the principle of environment interactions. This type of algorithm learning process does not require preparation of input data samples in contrast to the learning processes previously explained. It consists of three parts, i.e., *agent, environment* and *reward*, see Fig. 6 for more details. An action is performed by the agent at the current state, it moves to the next state and the environment feedback generates a reward for this action. The new value of current state is stored in the system based on the reward value. The reward process compels the agent to perform better actions thus improving the accuracy of the network. Currently, Q-learning [116] and SARSA [117] are two predominant algorithms used in this learning process. Here, Q-function is the state value and the reward is stored in the Q-table. The major difference between these two algorithms are the reward storage mechanism in the Q-table. The Q-learning algorithm stores the Q values based on the next action (on-policy learning) while the SARSA updates it by choosing the current action (off-policy learning).

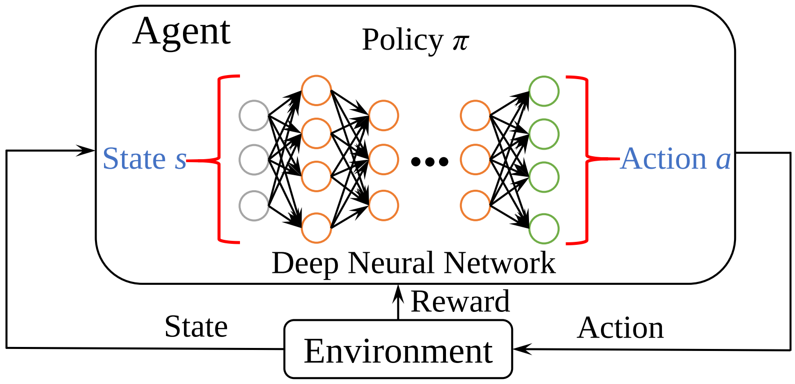


Fig. 6: Architecture of reinforcement learning.

For PnC and metamaterial designs, one needs to define the agent and environment carefully. The geometric and material parameters can be agent while the desirable response like band structure or frequency response spectrum are the environment. By altering the parameters one can change the system response. The trained model can then determine the structures that correspond to the optimization target. Recently, He et al.[114] adopted the Q-learning algorithm to enlarge the width of BGs in a phononic beam.

In short, the selection of any of this learning process greatly depends upon the problem type, desirable outcome, computational cost and accuracy. For both supervised and unsupervised learning are data-driven methods, we need an input database to train and test the network. Hence, if a larger dataset is involved, this may make the learning process computationally expensive. One can reduce the computational cost by tunning the hyperparameters of the NNs. Appropriate selection of the activation function is another important factor. As a result, while attempting to solve a given problem, it is important to get a dataset that is appropriate for the problem complexity and to validate the data distribution before applying it for model training. Further, during network training, one should be careful to not fall into a local optimum in the learning curve. This can be avoided by tunning and appropriate selection of hyperparameters.

5. Application of DL Processes in Metamaterials

5.1. Acoustic/Elastic Metamaterials

This section will cover a state-of-the-art review on the inverse design of PnCs and AMs/elastic metamaterials by ML and DL methods. We begin the development in this realm by discussing the ML method adopted for predicting the dispersion relation of one-dimensional PnC. Liu and Yu [118] developed deep back-propagation NN and radial basis function NN to predict the dispersion relation of one-dimensional PnC. The input dataset is generated by transfer matrix method to train the NN and detect the prediction accuracy. The reported results indicate good performance offered by both types of NNs and correctly predict the band structure for associated unit-cell structure of PnC. It is reported that for a single parameter prediction, the radial basis function NN performs well with a shorter training time. However, for multi parameter prediction, deep back-propagation NN have more stable performance. Later, for inverse design and BG magnification, Li et al. [83] applied MLP and CNN networks for the inverse design of two-dimensional PnCs. By using an image based finite element analysis along with MLP and CNN networks, Li et al. [83] studied design optimization of PnCs to broaden the BG width. The training and design of NNs are carried out at two stages as shown in Fig. 7. Initially, an AE is developed and trained to depict the topological feature of PnCs from randomly generated input design samples and by successful training of decoder network, the samples are reconstructed. The authors employed FEA to extract the band structure and frequency BG feature of PnC samples. The band structure of PnC is transported into the MLP network in the form of binary latent vector where 0 presents BG while 1 depicts passbands. Through a MLP network, the inherent relationship between frequency BGs and PnC topological features is established. Then the trained NN is utilised to search for the design of PnCs with anticipated BGs. The input data is generated by using an analytical function with random geometries. This study is based on the merging CNN and MLP networks for inverse design and optimization of PnCs to widen the frequency BG.

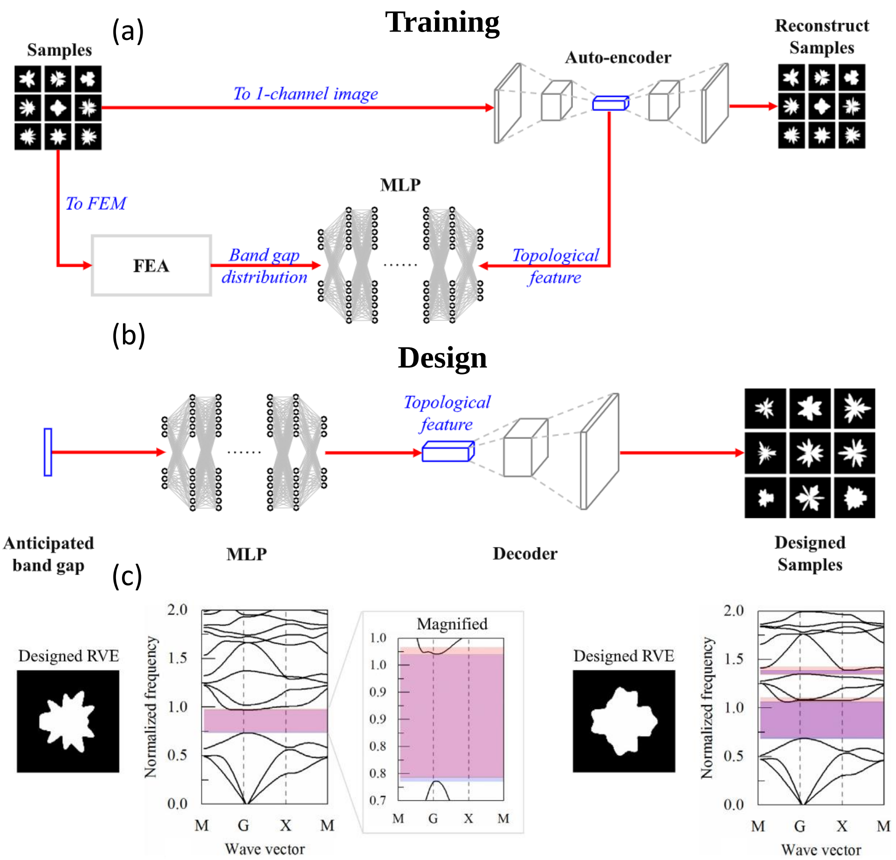


Fig. 7: (a-b) The training and design workflow for designing of PnCs with anticipated BG. (c) designed PnC with representative volume elements (RVEs). The figure is reproduced based on the results reported in Li et al. [83].

As explained in the prior section, GAN is another type of NN that works based on the principle of generator and descriptor networks. Since the early development, GANs have improved in many ways and applied in multiple applications like the design of an optical cloak [119]. Recently, Gurbuz et al. [84] applied the conditional GANs for an inverse design of AMs. They built a conditional GAN to derive geometric characteristics based on the target transmission spectra as shown in Fig. 8. The developed input database is based on C-shape resonators in a fluid environment. Based on this approach, FEA simulation is performed to calculate the frequency transmission characteristics for each sample and this information is linked with the discretized geometric shapes. After successful training, the GAN is able to induce transmission spectra for new AM geometries. To avoid high computation effort, the network is trained on a frequency range from 2 kHz to 10 kHz with a step size of 100 Hz. Although the frequency step is not fine enough as imposed by computation capacity, the application of GANs in AMs and research findings are encouraging. The developed strategy can be employed for designing acoustic and elastic metasurfaces and other types of AMs including topological insulators where structural features is required to be searched for desirable frequency response spectra.

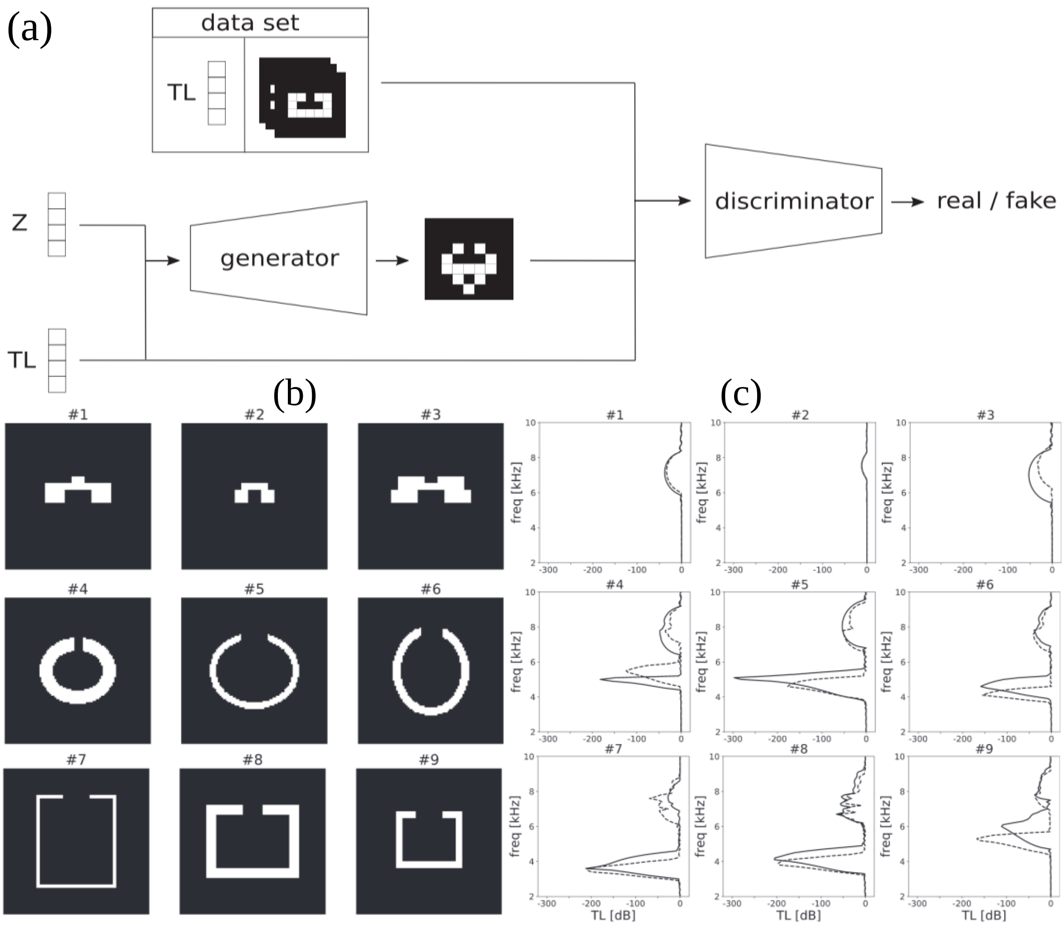


Fig. 8: (a) Architecture of GAN network adopted by authors. (b-c) Designed AM with predicted acoustic transmission loss using GANs. The simulated transmission loss of the designed cell candidate (solid lines) is compared with the input transmission loss from the databased (dashed lines). The figure is based on the results reported in Gurbuz et al. [84].

Assuming mechanical design as a *game* and in order to maximise the *score*, recently Luo et al. [120] developed RL network to design layered PnCs with anticipated band structures. Through an interactive RL technique, the topological structure of layered PnC is developed and it is allowed to evolve until it achieves a topological structure that satisfies the required specifications. For searching the BG of desired frequency range and optimizing the first-order BG width, it is found that the RL approach performs quite well. In another work, Maghami et al. [121] proposed deep RL to inversely design layered PnC beams with the required band structure and BG focusing on thermoelastic wave propagation. They used environment, agent and reward analogy to accurately capture the band structures and frequency BG regions for the layered PnC beam models. Likewise, Shah et al. [122] developed RL network for the inverse design of AM based on cylindrical scatterer in water medium. In another work, Maghami and co-workers [123] developed a data-driven PnC band structure prediction model to study nanophononic beam subjected to nano-size effect. They established computational intelligent method using data-driven DL tool to explore the design space of PnC subject to thermal shock loading. By using analytical formulation, an input dataset was established and DL network was trained. Later, the network efficiency was validated by comparing the DL network prediction with numerical simulation and excellent agreement was reported.

In order to optimize the band structure and BG of two-dimensional PnC, DNN with GA is adopted by Miao et al. [124] to accurately design PnC with anticipated BGs. Likewise, Wu et al. [125] developed two ML based techniques to design one-dimensional periodic and aperiodic AMs. For periodic AM designs, the RL based approach is proposed to achieve desirable frequency BG in a quick and computationally efficient manner. Because RL does not require a training dataset, this enables a quick and online AM design. For aperiodic AMs, the NN based approach is proposed to learn the behaviour of induvial unit-cell structure associated to frequency BG. A surrogate model of the entire AM samples is used to determine the properties of the final assembly by constructing the NN representation of individual unit-cell structure. It is interesting to note that the suggested method just needs one network training operation and it can mimic many AM assemblies while fulfilling user-defined parameters. To reduce the computational time for structural optimization of elastic metamaterials, Dong et al. [126] developed a surrogate modelling algorithm based on multilayer feedforward NN and Nelder-Mead algorithm. The NN is trained by ML method and optimization work is carried out by GA to increase the accuracy in predicting the location and BG width. The obtained result is compared with numerical FEA solutions and excellent agreement is reported. Likewise, Jiang et al. [127] developed DL network to map the band structure with structural topology of elastic metamaterials. The proposed network can inversely design elastic metamaterials based on the target band structure and BGs, see Fig. 9.

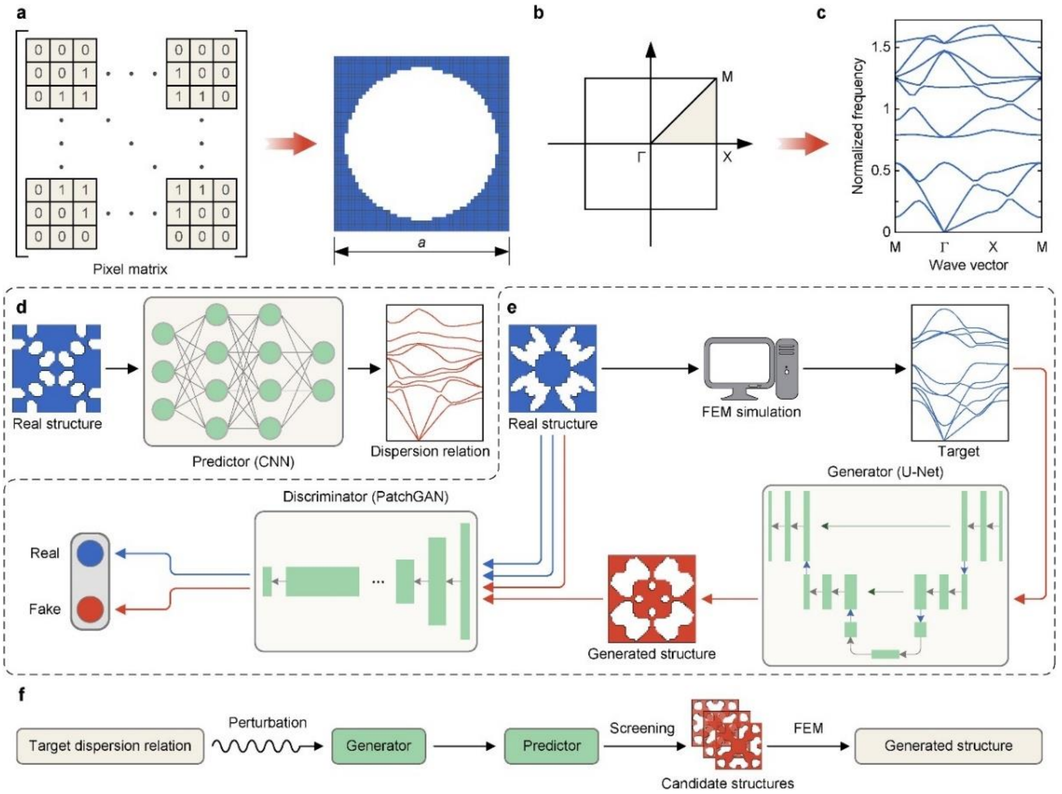


Fig. 9. Workflow for inverse design of elastic metamaterials by DL method proposed by Jiang et al. [127]. (a) Schematic of the pixel matrix and the unit-cell structure; (b) Brillouin zone of the square lattice; (c) dispersion relation calculated by FEA; (d) schematic of the CNN used for predicting the dispersion relation; (e) schematic of the cGAN used for unit-cell structure generation; and (f) proposed framework for inverse structural design. The figure is reproduced with permission from Jiang et al. [127].

In order to predict the presence and location of BG in PnCs, Sadat and Wang [128] developed a ML model as a smart and rapid screening tool. The developed tool can quickly capture the BG location, centre frequency and width. They tested three different ML algorithms i.e., linear regression, NN and random forests for this purpose and it is reported that the random forests performs the best. It is deduced that a random PnC has 17% probability to show frequency BG. However, with the random forest ML method, this probability shows a marked increase to 89%.

One challenge in the inverse design of AM with desirable physical response is the expensive iterative fitness evaluation by the traditional optimization methods. In order to overcome this problem, Chen et al. [107] developed a physics guided ML based inverse design model to realize multifunctional wave control in an active AM beam, name as the metabeam which connected with negative capacitance. Analytical formulation based on the transfer matrix method is obtained and MLP is trained to correctly map the input and output response of unit-cell structure, see Fig. 10 for more details. After successful training, the network performance is validated by comparing the predicted result with FEA numerical simulation. By treating the proposed network as a surrogate model for GA, they inversely design metabeam with multifunctionality without changing the microstructure.

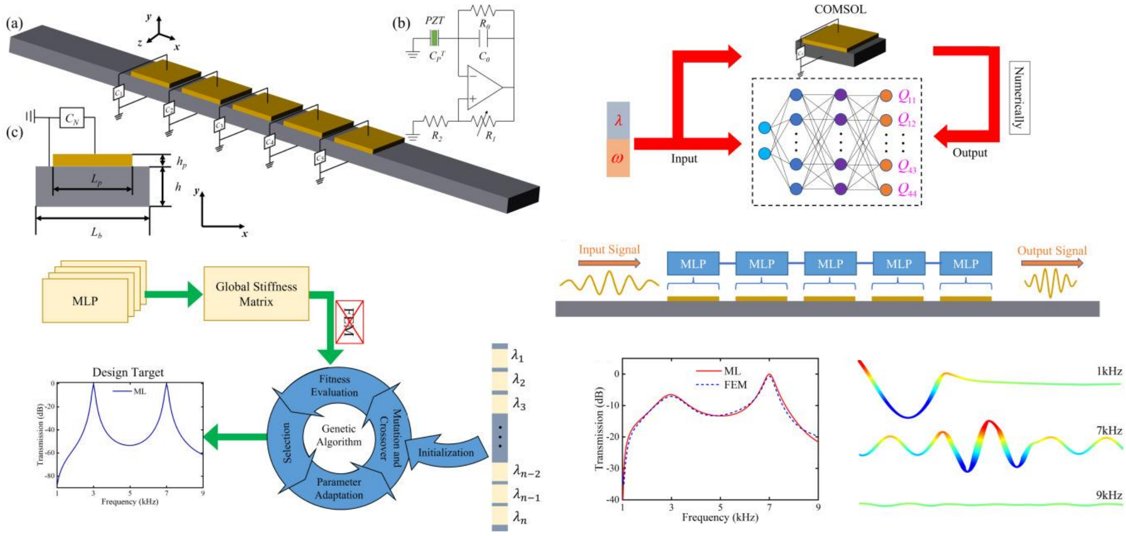


Fig. 10: Inverse design of multifunctional active metabeam proposed by Chen et al. [107]. The metabeam architecture, design optimization procedure and adopted methodology are shown. The comparison of DL based prediction and numerical results are also presented. The figure is reproduced with permission from Chen et al. [107].

Furthermore, He et al. [108] inversely design a metaplate with topological edge states for flexural wave control using the ML model. The input dataset is obtained by solving the metaplate dispersion relation by the plane wave expansion method. The ML network is trained and topological edge states are realized by the numerical simulation where direction selective flexural wave propagation is demonstrated.

Further, by applying probabilistic DL models, recently Ahmed et al. [129] inversely designed a broadband acoustic cloak to hide an object from incoming sound waves. AE like NN is deployed to retrieve material and geometric parameters of the cloak shell surrounding the object that suppresses sound scattering in a broadband frequency region. Reminiscent of optical and acoustic cloaks, the data-driven DL method is also found useful in the inverse design of mechanical cloak. A mechanical cloak is an arrangement of tiny structure blocks engineered in such a fashion that make an object invisible for any incoming elastic waves. Recently, Wang et al. [130] proposed a mechanical cloak engineered by DL methods using aperiodic randomly generated metamaterial design, see Fig. 11. The DL network is trained using a database of aperiodic randomly generated metamaterial designs. The network performance is validated by numerical simulations and performing experiment tests on the additively manufactured aperiodic designs.

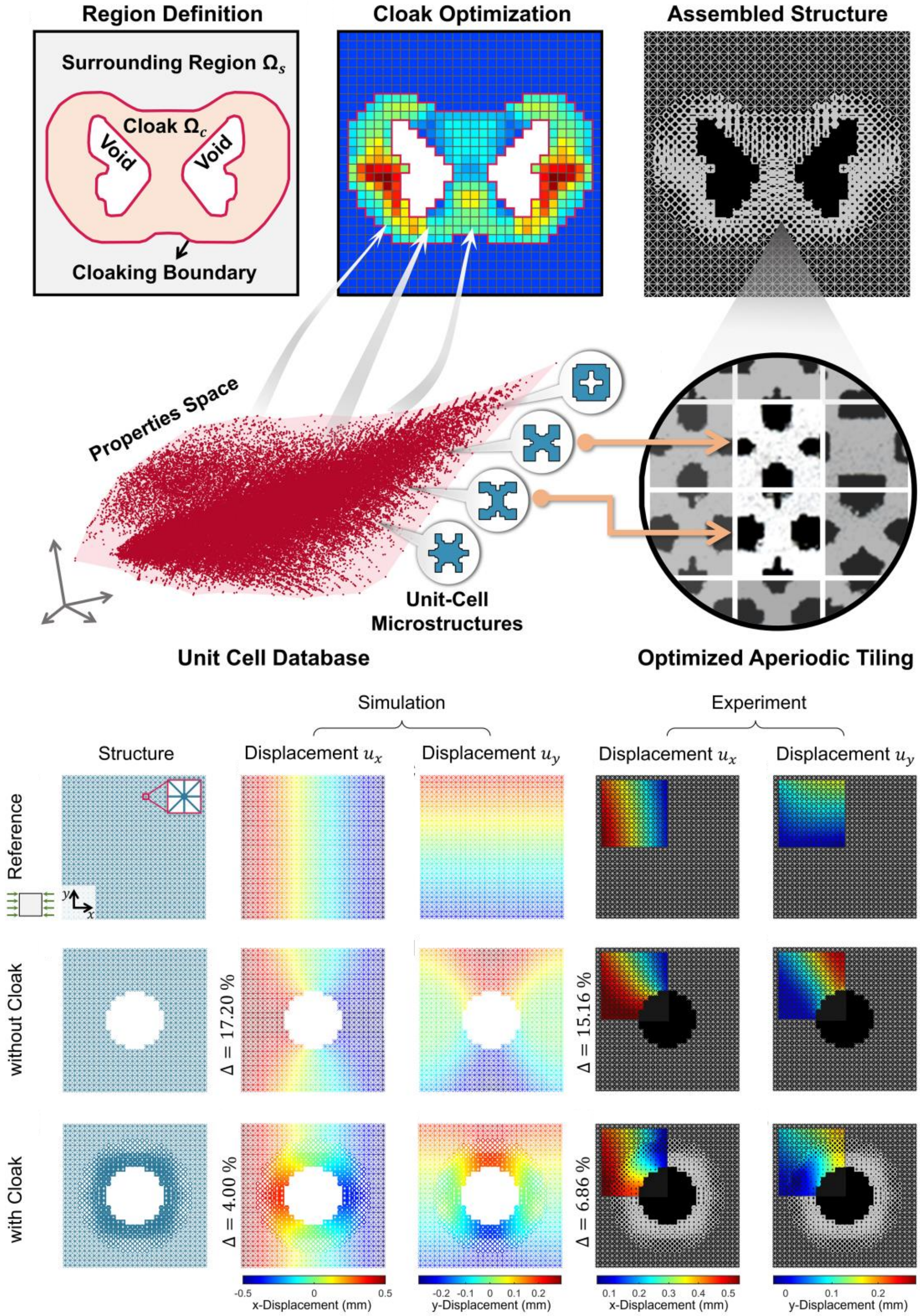


Fig. 11: Metamaterial aperiodic design based mechanical cloak: (top) schematic diagram of the data-driven approach; (bottom) comparison of numerical and experimental result

predicted by the DL networks. The figure is reproduced with permission from the Wang et al. Wang et al.[130].

Some applications of DL in the inverse design and optimization of AM for noise insulation have also been proposed. Donda et al. [109] applied CNN to design ultrathin acoustic absorbing metasurface that breaks the quarter wavelength resonator theory and absorbs sound wave at deep subwavelength scale, see Fig. 12 for details. The total path length inside the metasurface channel for propagating sound wave is $\lambda/5.7$ and the proposed metasurface can absorb the acoustic wave at extremely low frequency. The CNN results are compared with other types of optimization approaches and further validated by experiment tests. By combing multiple unit-cell structures, a supercell array of the metasurface is designed to broaden the absorption frequency range. Similarly, Zheng et al.[72] developed the ML method using a Gauss-Bayesian model to inversely design AM for perfect sound absorption at specified frequency and ensuring air ventilation. During the design process, physical parameters are adjusted inversely from the sound absorption coefficient at a desirable frequency range with limited calculation. The interaction between sound wave and resonators ensured good sound absorption at a low-frequency region. The sound absorption performance is verified by numerical simulation and experiment test. For acoustic optimization, one can refer to Bianco et al. [131] for ML in acoustics with theory and applications and the pioneering work of Marburg [132] on acoustic structure optimization techniques.

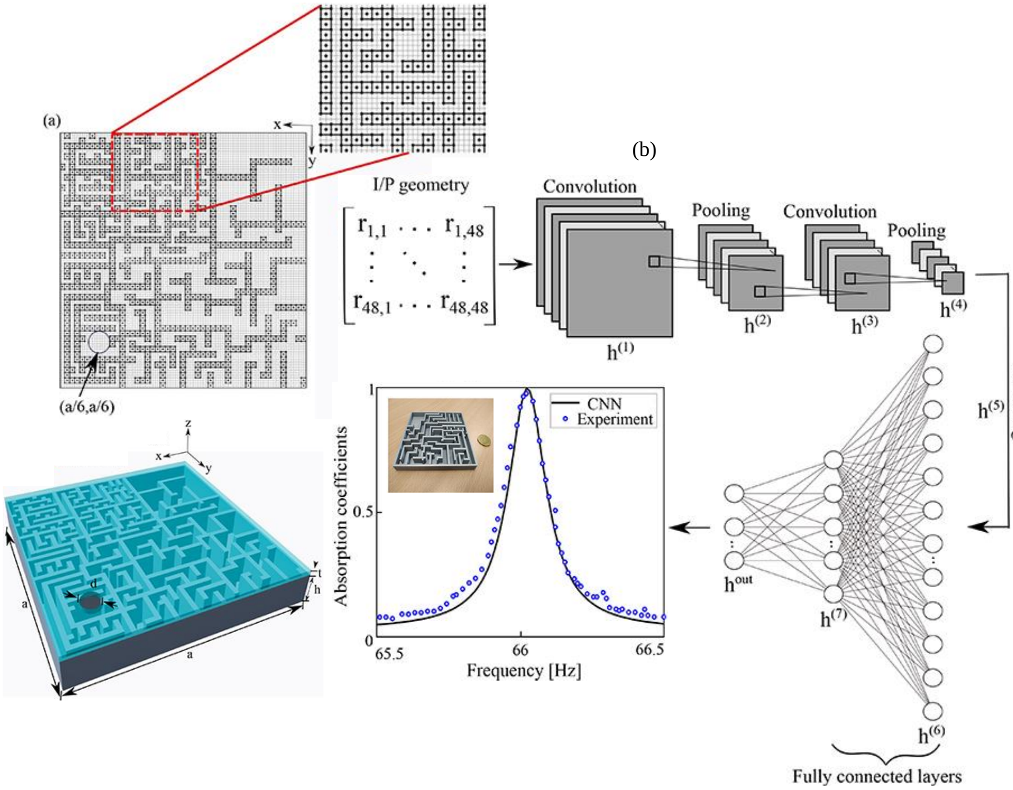


Fig. 12. (a) Schematic illustration of matrix encoding; (b) DL network architecture developed for design optimization and performance enhancement of ultrathin metasurface absorber. CNN is fed to a collection of geometric inputs, which rearranged and upsampled the data in a learnable way. The CNN output is passed to the fully connected layers that provide a predicted spectrum (red dashed line) that is compared to the ground truth (blue solid line). The figure is reproduced with permission from Donda et al. [109].

5.2. Mechanical Metamaterials

Apart from acoustic/elastic metamaterials, bioinspired hierarchical composite design is another emerging research topic that has found strong roots in mechanical metamaterials. Mechanical metamaterials are functional structures with extreme static mechanical properties. Biomimicry, which involves adopting and applying nature's design, is an effective first-order approach to obtain superior mechanical characteristics. However, the design space is too vast for optimization even using biomimetic design prototypes. In that context, Gu et al. [133] proposed a new strategy for designing hierarchical materials that combine ML. The model was trained on a database comprising hundreds of thousands of finite element structures, with a self-learning algorithm for discovering high performance materials. As a result, inferior designs are phased out in favour of superior candidates. This trained ML algorithm has generated new designs that are validated through additive manufacturing and experimentation. The CNN model is augmented with a self-learning algorithm which learn data patterns from sampled top-performing geometries to create even better designs by excluding the inferior designs. The search for rare mechanical metamaterial designs that will lead to highly unusual material properties and mechanical behaviour like high elastic moduli and double-auxeticity remains an important task. Recently, Pahlavani et al. [110] developed a computational model and DL algorithm to identify such rare mechanical metamaterial designs from a large dataset. Specifically, they studied the relationship between random distribution of soft and hard interfaces in three types of planar lattices and their mechanical characteristics by two-dimensional DL networks. The developed algorithm and computational model can quickly map the mechanical properties with a vast design space and quickly give desirable design output, see Fig. 13 for more details.

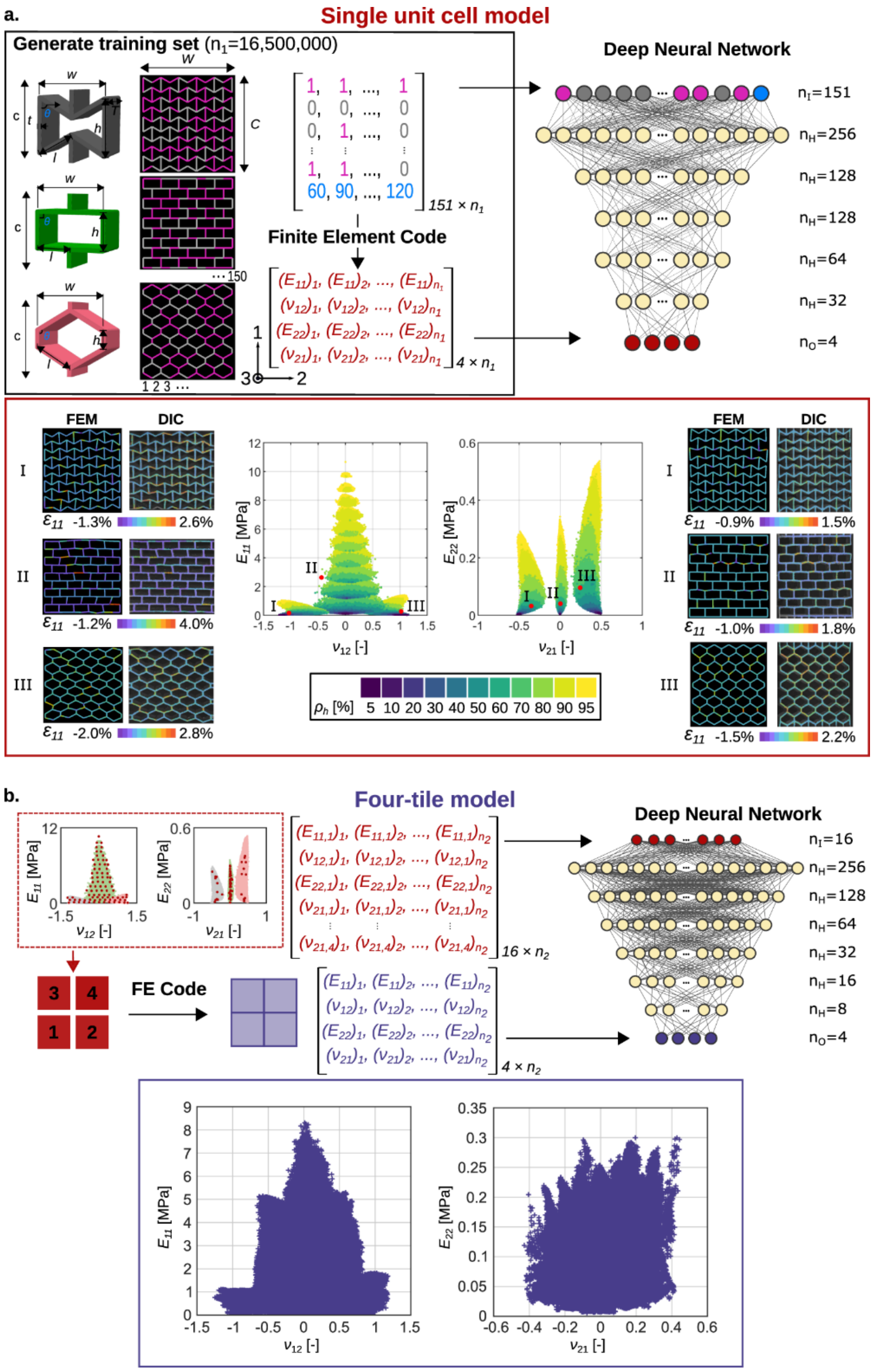


Fig. 13: Inverse design of mechanical metamaterials. The structures of optimized deep learning models, the relevant training procedures and the range of attainable mechanical properties are shown. The figure is reproduced with permission from Pahlavani et al. [110].

Because of their bistability property, curved beams have been widely employed in energy absorption materials and MEMS systems. The previous designs of such beams were carried out by shape optimization approaches. Recently, ML is recognized as an effective approach for the design of curved beams [111], see Fig. 14. This method can predict highly accurate mechanical nonlinear structure properties. Different optimization targets, such as stiffness, forward snapping force, and backward snapping force, are effectively and precisely obtained.

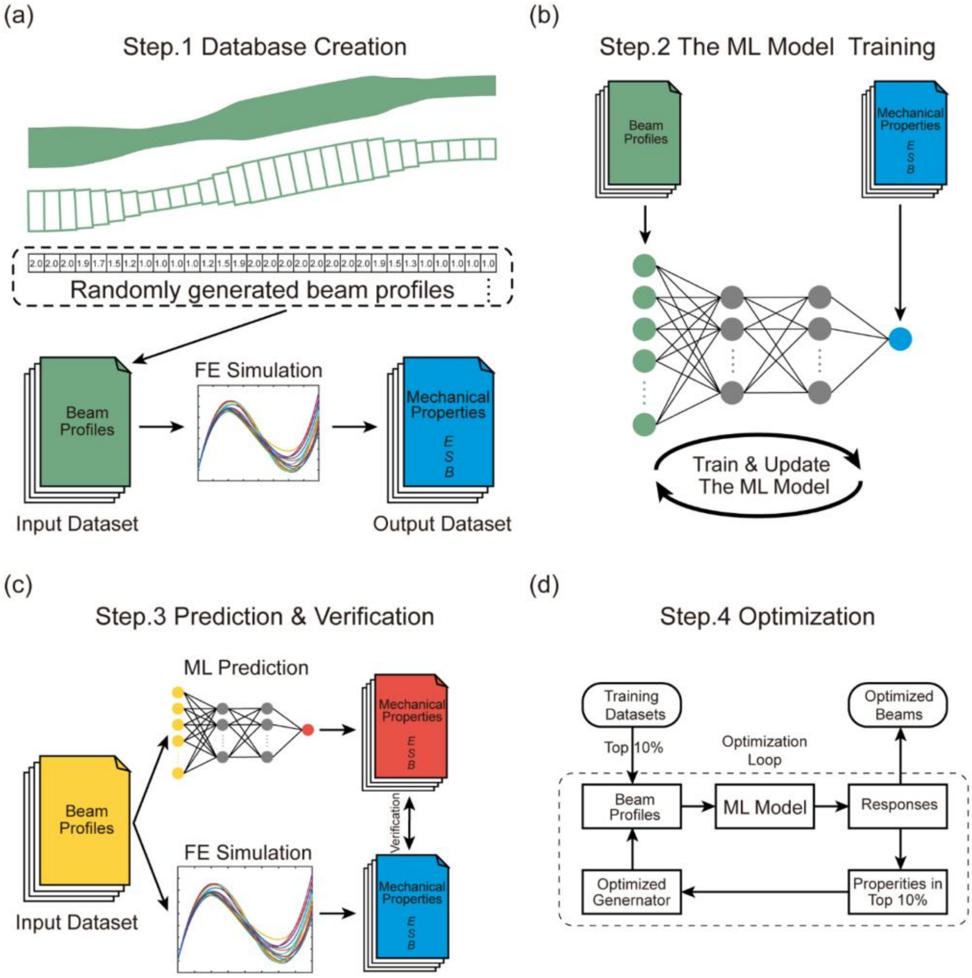


Fig. 14. The 4-step ML process for design optimization of a curved beam; (a) input database; (b) training process; (c) ML prediction and model validation; and (d) optimization flow chart. The figure is reproduced with permission from Liu et al. [111].

Other challenges involved in the design optimization of mechanical metamaterials include high-dimensional topological design space, multiple local optima and high computation costs. Recently, Wang et al. [112] reported a unique data-driven metamaterial design approach based on deep generative modelling to overcome these challenges. To map complicated microstructures into a low-dimensional, continuous, and structured latent space, a variational AE and a regressor for property prediction of mechanical metamaterial are simultaneously trained on a large database. Here they illustrated how the variational AE latent space can be used to calculate shape similarity, interpolate across microstructures, and encode significant patterns of variation in geometries and properties. Based on these findings, systematic data-driven techniques for microstructure, graded family, and multiscale system design are presented. By a simple vector operation in the latent space, the tunning of mechanical properties and manipulation of microstructures was achieved. By searching on a developed graph model, the vector operation is extended to produce mechanical metamaterial families with a controlled gradation of mechanical characteristics. A diverse collection of microstructures was produced using variational AE for the desired characteristics at different locations for multiscale metamaterial systems design. It is then integrated using an efficient graph-based optimization approach to assure compatibility between adjacent microstructures, see Fig. 15 for more details. We believe that the mechanistic insights gained in this work can be applied to general microstructural materials since the meaningful latent space is a result of its continuity and low dimensionality. Possible future applications of the proposed research methodology include the design of 3D mechanical metamaterials. This will enable the variational AE to create 3D microstructures utilising sophisticated ML methods like 3D voxels or point cloud representations to be applied for 3D cases. Furthermore, since homogenized property calculations for 3D mechanical metamaterial is computationally expensive, a more advanced database creation approach is needed. These are some possible directions in the context of variational AE that will be the focus of future research.

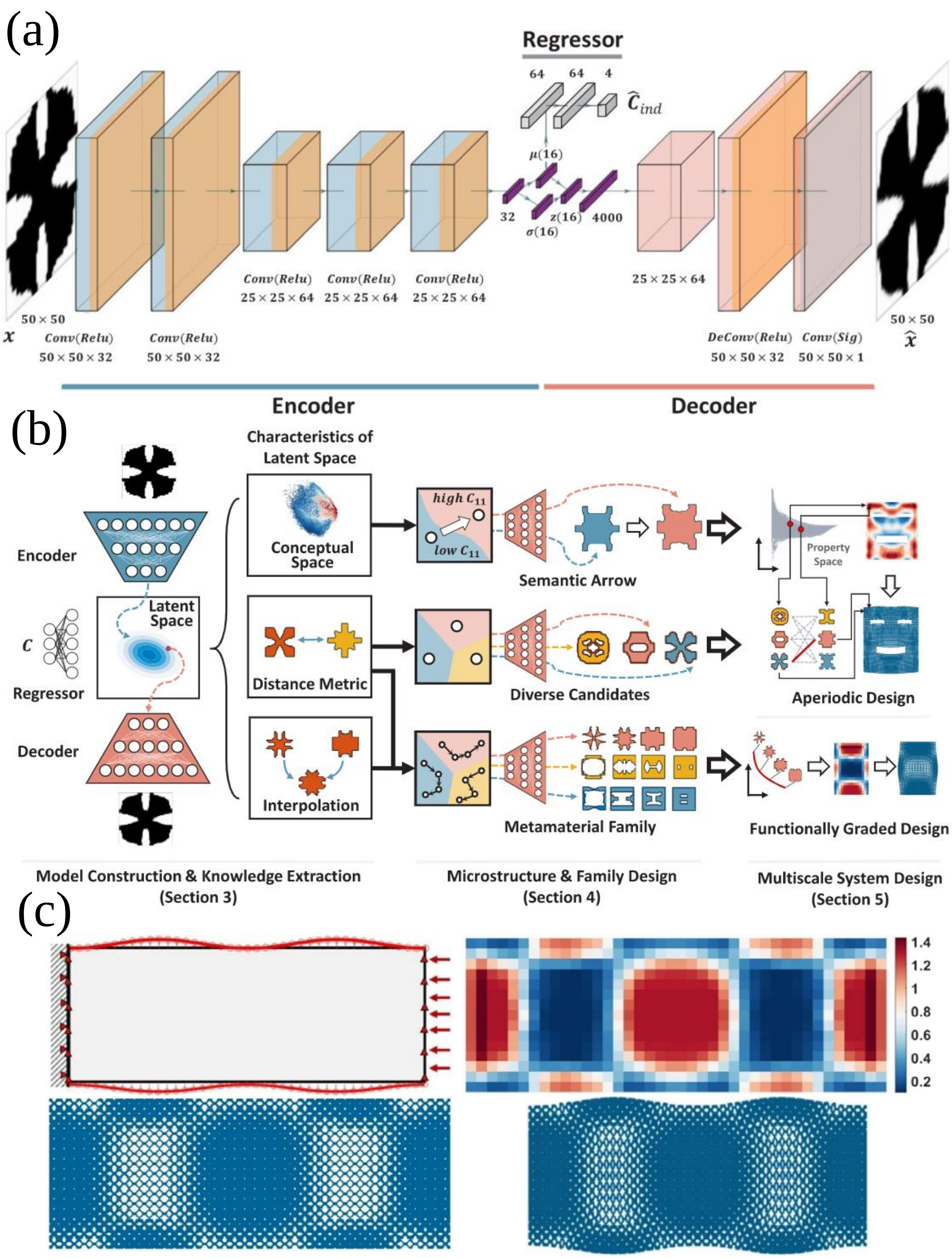


Fig. 15: (a) Architecture of proposed neural network; (b) VAE mechanistic-based learning and design of metamaterials proposed by Wang et al. [112]; (c) Target displacement and output design results for the first design case. The figure is reproduced with permission from Wang et al. [112].

To combat the costly physical simulations and to provide a pathway to efficient design of metamaterials, Chan et al. [134] developed METASAT, a twostep mechanical metamaterials design strategy. First, the closeness of unit-cell structures in both shape and property spaces are measured by using similarity metrics and positive definite kernels. Second, Determinantal

Point Processes are used to pick the subsets efficiently. The data-generation and design optimization strategy based on DL networks are performed on both 2D and 3D structures.

Auxetic structures exhibit non-natural negative Poisson ratio property. For inverse designs of auxetic structures, Wilt et al. [135] developed a DL model to facilitate quick design of mechanical metamaterials with less computational load. In order to train a regressive model and forecast the deviation from optimal behaviour, pseudorandomized pictures and the corresponding computational deformation results are applied. They also compared the DL predicted results with numerical simulations. Likewise, Ma et al. [136] proposed deep learning accelerated inverse design of mechanical metamaterials by adopting the magneto-mechanical actuation technique, see Fig. 16 for more details. Compared to conventional metamaterials, this new class of active structures can tune their mechanical properties without altering the structural properties.

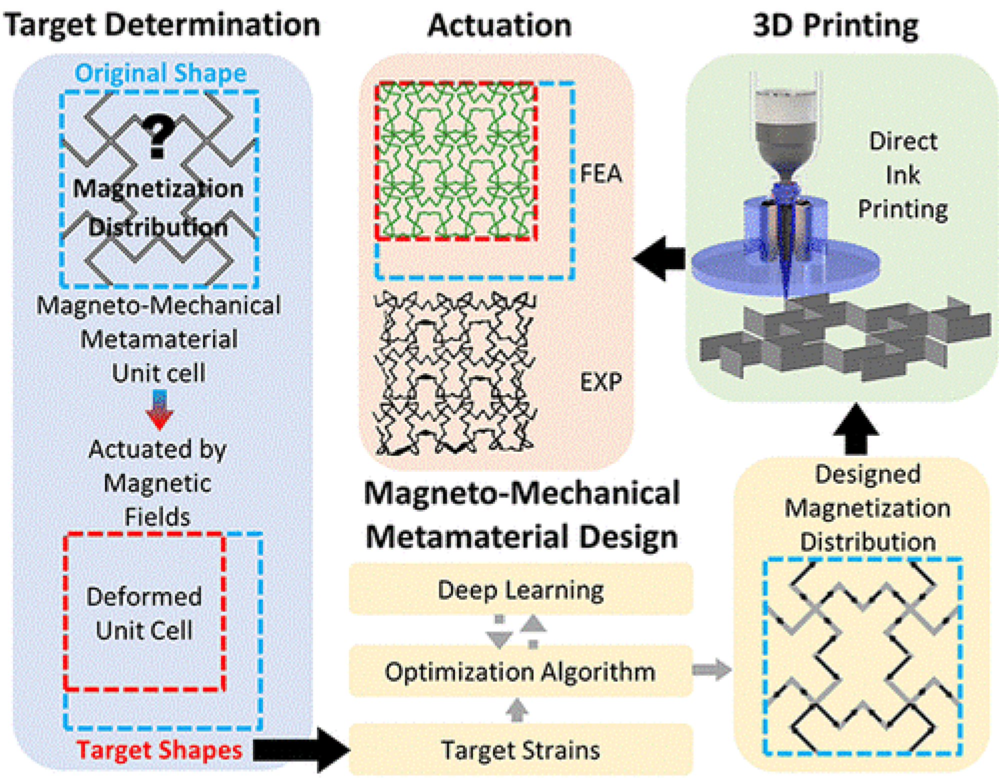


Fig. 16: Deep learning based accelerated inverse design of magneto-active mechanical metamaterials. The figure is reproduced with permission from Ma et al. [136].

6. Limitations and Recommendations

As a subset of AI, machine learning (ML) and deep learning (DL) are data-driven methods that have covered a wide range of disciplines like pattern recognition, computer vision, natural language processing, material science and engineering, etc. These data-driven methods are straightforward codes that execute algorithms for parsing and learning from the input dataset. Hence, ML and DL are algorithms that work based on the principle of statistics/regression to correlate input parameters with output results. While these methods are being investigated by researchers in a wide range of disciplines, the potential outcomes are not equally promising. The algorithms that efficiently learn pattern recognition, image classification in computer vision and natural language processing, may not be ideally promising for physics, mechanics and material science problems. In those problems, partial differential equations using computational tools such as finite element method, boundary element method are used to predict solutions. To date, these equations and computational tools are extensively used for investigations on phononic crystals and metamaterials. Contrastingly in ML and DL methods, algorithms that are unaware of those equations and governing physics have established a functional relationship between input data and output results. Some of those examples are covered in this review. ML and DL methods use the least square method to establish functional relationship by fitting the parameters. Therefore, these data-driven methods perform simply least square fitting of input data in a hyperdimensional space, at least this is what observed in the literature.

Looking at the surge of research studies on particular topic of this review, careful consideration is needed to answer the following queries. (i) Is it worth applying ML and DL methods to solve particular phononic crystal and metamaterial problems? (ii) If so, what will be the requirements, challenges and bottlenecks? In order to answer these questions, a thorough understanding of the fundamentals of the ML and DL methods and the related governing physics and engineering concepts are required. Several studies have reported that these data-driven techniques will make the phononic crystal and metamaterial designs independent of numerical computation. This demonstrates that an established algorithm can give efficient designs which are correct for the specific problem but it may not be generalisable. Another big challenge concerns the process of generating input data that is used to train and test the algorithms. If one considers the computational cost for data generation and training the DL algorithms, the amount of time and resources required will be equivalent to, or for some problems even more than, what is needed for the conventional approaches. In order to train the networks, thousands of data samples must be generated using a rigorous analytical model, numerical simulations and sometimes a large number of experiment tests. Hence, the computational effectiveness of these data-driven method is frequently questionable. To some extent, this challenge can be minimised by applying Monte Carlo sampling, SOBOL sequence and Latin hypercube methods. These methods also facilitate in selecting optimal sample size that helps in reducing computational cost for data generation and sampling. Such techniques together with ML models have been applied in a number of studies [137-142]. It is anticipated that, those techniques together with ML and DL methods may find useful application in phononic crystal and metamaterial research.

Another issue concerns the hyperparameter tuning of ML and DL networks. This includes the number of hidden layers, the number of neurons in each layer, the type of activation function, learning rate, number of epochs, etc., needed to train the algorithm efficiently and successfully. After data generation that involves considerable computational resources, tuning hyperparameters of network is another resource problem that needs to be resolved. A set of hyperparameters that work very well for one particular problem may give poor performance for another problem. Reminiscent to the input data, hyperparameters do vary from a problem to another. For example, in computational mechanics problems with a major change in geometric parameters and initial boundary condition(s), a separate network needs to be established and retrained. This problem can be minimised possibly by using simultaneous training-testing algorithms like k-fold cross validation, hold-out cross validation, leave one out (LOO)/ leave p out (LPO) cross validation etc. methods. Further details about the cross-validation frameworks in ML and DL can be found in [143-145].

In short, the answers to the following questions are required prior to applying ML and DL methods in phononic crystal and metamaterial problems:

- What will be the cost for data generation?
- What resources are required for generating input data and algorithm training?
- What will be the cost of training a neural network?
- How to effectively tune the hyperparameters that can be easily deployed for a number of other seminal problems?
- What methods can be used to avoid over-fitting and under-fitting of data?
- How much data is necessary to train a network efficiently and successfully?

After training and testing, for network prediction, the answers to the following questions are important:

- Can the output give an accurate prediction for physical parameters beyond the range considered in the input database?
- How to develop and train a generalized network which is able to adapt to changes in geometry, initial conditions, discretization etc?

- What are tolerances and margin of errors for the input parameters? What is the sensitivity of the network to variation in input parameters for a given error margin?

7. Summary and Future Prospects

Machine learning and deep learning has evolved from a computational analogue of biological brain networks to a strong tool for solving highly complicated problems by constructing layered abstractions from large amounts of data. These approaches are currently revolutionizing the field of material/structure design, integration and measurement for the acoustic and mechanics communities. Deep-learning techniques have already demonstrated their enormous potential for phononic structure design, optimization of architecture, mechanical metamaterial designs, material optimization in the entire acoustic and elastic systems, and will continue to uncover new ways to accelerate inverse design, optimization and potentially result in the discovery of new physical effects.

On one hand, during the past two decades, an enormous amount of research interest in artificial materials is witnessed, these are the so-called phononic crystals, acoustic/elastic metamaterials and mechanical metamaterials/architected materials with evident discoveries. On the other hand, we also observed rather rapid advancements in the machine learning and deep learning techniques. Recently, these two research streams have merged and formed another multidisciplinary research field with enormous opportunities for both fundamental research to resolve the present challenges and to pave the way for real-life engineering applications. This was enabled by the advancements in computer science and electronics that provide researchers with state-of-the-art hardware support. The intersection of these two diverse fields will provide researchers a substantial range of opportunities to solve the present challenges, especially in the inverse design, optimization and performance improvement fronts. The successes in these areas are expected to result in revolutionary developments in the near future.

This review article has covered a variety of model structures for phononic crystal, acoustic/elastic metamaterial and mechanical metamaterial designs that range from optimization of individual unit-cell structure to supercell arrays with fascinating results. All of these extraordinary advancements have occurred in the last few years, and more are predicted as scholars from all disciplines contribute to this developing subject. The basic network types, learning processes, network architecture and their governing principles are covered that can help readership have a thorough understanding for fostering future research.

In order to develop novel, physics-driven algorithms and networks that are not only reliable, generative, and interpretable while using less data, but also to offer novel ways to achieve unrivalled acoustic and mechanical functionality, deep learning researchers should work with acoustic and mechanical scientists. Such collaborations will eventually merge AI with material science, acoustic and mechanic communities and enable the designs and real-life applications of metamaterials with unique functionalities. On this track, the material science, acoustic, physics and mechanic groups should establish a comprehensive dataset of phononic crystal and metamaterial concepts, topologies, components, and materials to allow hierarchical machine-learning algorithms that could offer ultimate-efficiency devices.

Appendix

Fully connected neural network

As discussed in the supervised learning, a fully connected neural network with *N* layers consists of an input layer, output layer and *N*-2 hidden layers. These neurons are interconnected i.e., each neuron in the input layer is connected with all neurons in the next layer without any interlayer connections. Layer after layer, the neurons analyse the incoming data using learnable parameters such as weights (*w*) and biases (*b*). Assuming the weight of the n^{th} neuron in the (m-1)$^{\text{th}}$ layer to the k^{th} neuron in the m$^{\text{th}}$ layer as w_{jn}^{m} and n^{th} neuron has bias b_n^m, the output for the n^{th} neuron in the m^{th} layer will be a_n^m that is calculated by summation of weights from the previous layer with the help of some nonlinear activation function $\sigma(\bullet)$, assuming the previous layer is p_n^m. Instead of degrading to a basic linear mapping, $\sigma(\bullet)$ allows the network to handle very complicated data representation. Some popular activation functions are sigmoid, ReLU, hyperbolic tangents. As a result, the input data is transferred from one layer to the next in the forward process, being linearly summed and nonlinearly triggered at each stage, much like the electrical signal flowing through biological neurons and synapses. Mathematically, it can be expressed as

$$a_n^m = \sigma\left(\sum_k w_{nk}^m a_k^{m-1} + b_n^m\right) = \sigma\left(w^m a^{m-1} + b^m\right) = \sigma\left(p_n^m\right) \quad (1)$$

In term of matrix and vector notations, the weights and bias in the *m* layer is $w^m = \left(w_{nk}^m\right)|_{1\le n\le|n|,1\le k\le|k|}$ and $b^m = \left(b_n^m\right)|_{1\le j\le|j|}$, respectively. To estimate the network performance and error, a cost function $C(\bullet)$ is defined that compares the output results with ground truth. This is minimized by adjusting the weights and bias in each layer by calculating the gradient.

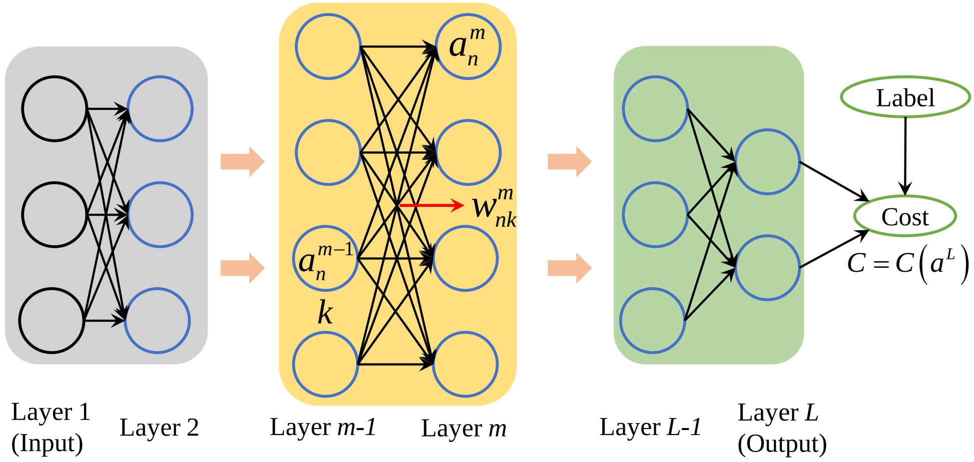


Fig. A1. Architecture of deep neural network with weights and bias parameters.

Back-propagation algorithm

The back-propagation method, which is a practical implementation of the chain rule for derivatives of a multivariate function, is used to train a neural network with only one backward pass from the output layer to the input layer. Assuming an intermediate error vector $\delta^l = (\delta C/\delta p_1^1, \delta C/\delta p_2^1, \delta C/\delta p_3^1 ...)$ that is actually the partial derivative of the cost function C with respect to the weighted input in the layer l, hence, the error in the last layer will be

$$\delta^L = (\nabla_a C) \odot \sigma'(z^L) \tag{2}$$

where $\odot$ is the Hadamard product that shows an elementwise product of two vectors. Since the activation function $\sigma(p^L)$ and cost function $C(a^L)$ have analytical forms, therefore δ^L from the last layer can be obtained. Likewise, with the help of the partial derivative chain rule, the error vector of layer l i.e., δ^l (other than last layer) can be calculated from errors of the next layer δ^{l+1} using

$$\delta^l = \left[(w^{l+1})^T \delta^{l+1} \right] \odot \sigma'(z^l) \tag{3}$$

Eqs. (2-3) shows the main idea of back-propagation algorithm. The cost initially calculated by quantifying the discrepancy between output layer and target/ground truth data backflows from the last layer to the first layer by calculating intermediate error of each layer.

$$\frac{\partial C}{\partial w_{nk}^l} = a_k^{l-1} \delta_j^l ; \; \frac{\partial C}{\partial b_j^l} = \delta_j^l \tag{4}$$

Based on Eq. (4), the network can be trained by the stochastic gradient descent where the training data is mixed and divided into batches where each batch contains a small amount of all data. The training process includes, feeding the input data to the network, calculating the output and quantifying the errors. Then by using the back-propagation approach, the weights and bias are calculated and the cost function is adjusted at each layer. For the network learning process, a hyperparameter η is defined that controls how much weights and bias need to be modified as a portion of the gradient with respect to the cost in that particular batch. Assuming a batch has M training data, then according to Eq. (4), the updated rules are

$$w^l \to w^l - \frac{\eta}{M}\sum_x \delta^{x,l}\left(a^{x,l-1}\right)^T ; \; b^l \to b^l - \frac{\eta}{M}\sum_x \delta^{x,l} \tag{5}$$

The training step is repeated several times until the cost value no longer decreases. Once the training process is complete, the network performance is cross-checked by different tests with samples that were not available in the input data for training.

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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.

CRediT authorship contribution statement

Muhammad: Main idea, Conceptualization, Methodology, Formal analysis, Investigation, Literature survey, Writing-original draft, Visualization, Validation, Project administration. **John Kennedy:** Investigation, Funding acquisition, Writing – review & editing, Project administration, Resources, Supervision. **C.W. Lim:** Investigation, Writing – review & editing, Supervision.

Data availability

The data that supports the findings of this study are available from the corresponding author upon reasonable request.

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