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Hybrid inverse design of photonic structures by combining optimization methods with neural networks

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ABSTRACT

Over the past decades, classical optimization methods, including gradient-based topology optimization and the evolutionary algorithm, have been widely employed for the inverse design of various photonic structures and devices, while very recently neural networks have emerged as one powerful tool for the same purpose. Although these techniques have demonstrated their superiority to some extent compared to the conventional numerical simulations, each of them still has its own imitations. To fully exploit the potential of intelligent optical design, researchers have proposed to integrate optimization methods with neural networks, so that they can work coordinately to further boost the efficiency, accuracy and capability for more complicated design tasks. In this mini-review, we will highlight some representative examples of the hybrid models to show their working principles and unique proprieties.

1. Introduction

Mimicking the operations of animals' brain activities such as recognizing the features of objects from different classes, artificial neural networks, or simply neural networks (NNs), form the backbone of the deep learning algorithms [1–4]. In a typical neural network, data pass through successive layers. The weights of nodes, or so-called neurons, in each layer are updated iteratively through the forward and back propagation procedure, completing the training process of NNs. Recent studies have shown that with the ability to learn the features from the training dataset, NNs can perform forward prediction and inverse design of various photonic structures, creating an exciting paradigm at the intersection of photonics and artificial intelligence [5–9]. For the forward prediction, the properly trained NNs can substitute the conventional time-consuming numerical simulation, since NNs can easily and accurately predict the optical response once the geometries and or material distribution are given. For the inverse design, NNs function in the opposite way. In other words, NNs can retrieve the optimal structure in order to achieve specific target responses or functionalities. These tasks might be very complicated and challenging by conventional parameter-sweeping-based design methods. Different NNs including fully connected neural networks [10–14] and convolutional neural networks [15–18] have been used in the photonic design, depending on the objectives and dimensions of the input/output parameters. Applications such as multi-band absorbers [19], chiral metamaterials [20], near-/far-field prediction [21], and vector field generation [22] have been successfully demonstrated.

Although NNs can effectively assist modern intelligent photonic design, they still have their limitations. For instance, we need to carefully select the configuration of NNs based on our expertize or empirical knowledge when dealing with specific applications. Moreover, large datasets, which are usually produced from intensive numerical simulation, are required for the training process. On the contrary, traditional inverse design approaches, such as adjoint-based topology optimization and genetic algorithms, have inherent drawbacks like time-consuming numerical calculations or simulation processes, although they have been used in a variety of applications. As shown in Fig. 1, it is of great interest to build hybrid models by combining NNs with other classical optimization algorithms, so that we can overcome their respective limitations, handle complex problems, and enhance the performance of the final design. Indeed, over the past years, people have devoted substantial efforts to explore this new direction. The research findings show that there are several advantages of such a hybrid approach.

(1) Conventional optimization methods can help to enhance or optimize the NNs including the training dataset, the structure of

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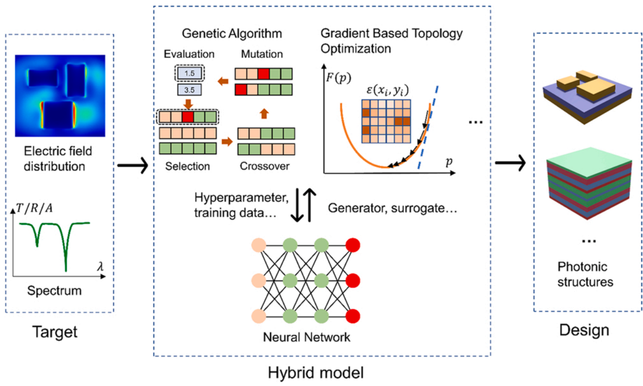

Fig. 1. Illustration of the workflow of combining classical optimization methods with neural networks.

the network, hyperparameters, and even the weight updating process. These factors determined the final performance of the NNs. However, the setting of them is always based on experience or laborious modification. With the help of optimization methods, the efficiency and accuracy of the NNs can be enhanced without manual interference.

(2) NNs can serve as an extremely fast electromagnetic solver in the inverse design process based on different optimization methods. For conventional optimization, time-consuming full-wave simulations are often required in each iteration. However, this step can be replaced by well-trained NNs to greatly accelerate the running time while maintaining high prediction accuracy. Previous works have adopted this method and demonstrated orders of magnitude speedup.

(3) The model may gain more advantages from the combination of optimization and NNs in a complex way. In some works, the optimization algorithm and NNs would function and update at the same time during the iteration precession, meaning that they would mutually benefit each other. For example, genetic algorithm (GA) can help to select better solutions that can be used in the training dataset while the NNs will learn from the optimized dataset and update the forward and inverse model with better accuracy. In this way, we can generate comparable results but with much smaller training data.

In this review, we will provide specific examples that combine optimization algorithms with NNs and discuss in detail their impacts on the final performance of the model and the device, in order to help the readers to better understand the three major advantages of the hybrid models mentioned above. The remainder of the review is organized as follows. In Section 2, we will discuss inverse photonic design by combining topology optimization (TO) and adjoint methods with NNs. In Section 3, we will show how to optimize the performance of NNs by introducing GA, a widely used non-gradient-based algorithm, to the hybrid model. Some other non-gradient-based inverse design approaches, including the Bayesian algorithm and Gerchberg–Saxton algorithm, in conjunction with NNs will be discussed in Section 4. We will cover the fundamentals of the specific hybrid methods and highlight the representative examples that exhibit exceptional performance when the optimization approach and NNs are combined. Finally, we will provide a summary and briefly discuss the future prospects in the conclusion section.

2. Fusing topology optimization and adjoint method with neural networks

TO is one of the most frequently utilized approaches for inverse design based on gradient descent [23–30]. The topology of the photonics device, which specifies the material distribution p_i for each pixel inside the design region, needs to be optimized to fit the target function F to the greatest extent during such process. An initial set of the input parameters are provided by the model, then the information of the gradient, i.e., $\partial F/\partial p_i$, can be obtained by electromagnetic simulation. Intuitively, a number of simulations (linearly scaled with the parameter number) need to be performed to reveal the gradient for the current parameter set, which are time-consuming and computationally expensive. However, this step can be accelerated by the adjoint method, where only one forward and one adjoint simulation are needed regardless of the amount of the parameters. Applications of TO in the design of wavelength demultiplexer [23], photonic crystals [24], and metagratings [25] have been demonstrated in recent years thanks to the merits of the adjoint method. In this section, we will discuss how TO and adjoint method can help to advance the development of NNs and vice versa.

Owning the ability to optimize the device performance by adjusting material distribution, TO can potentially improve the quality of the training dataset and even the post-processing of NNs. For instance, Z. Kudyshev and co-workers have recently proposed to merge TO with NNs to realize high-efficiency thermal emitters, which comprise plasmonic nanostructures based on transition metal nitrides [31]. Their approach shows greatly enhanced performances, including 4900 times faster optimization search, and maximum efficiency of 98% compared to 92% from the direct TO method. The top panel in Fig. 2**a** illustrates the model framework. An adversarial autoencoder (AAE) network, which can be regarded as a combination of variation autoencoders (VAEs) and adversarial learning such as generative adversarial networks (GANs), is applied to compress the pre-optimized input pattern into the 15-dimensional latent space and generate highly efficient designs from randomly sampled latent variables. The workflow of this optimization process mainly consists of three steps. First, the gradient-descent-based TO is applied to generate data for the training dataset. Then, the optimized patterns are sent to the encoder to compress them to the latent space, similar to the data compression process that can shrink the data from a higher to lower-dimensional space in VAEs. Since a large dataset is needed for the training process but the TO of each design is realized by the adjoint method that requires two time-consuming finite-difference time-domain (FDTD) simulations, the author augment the data from 200 to 8400 by considering the translation and rotation of the original structures. The discriminator then forces the latent distribution to fit the predefined distribution and the encoder generates a large set of designs from the latent space. In the end, the generated structures are refined by additional TO to eliminate sub-precision features as well as low-efficient and unstable designs. The authors suggest using pre-trained CNN, which can be regarded as a smaller version of VGGnet, to filter appropriate designs in order to accelerate the refinement. The comparison between the conventional cylindrical structure, direct TO, and AAE + TO can be found in the three figures at the bottom of Fig. 2**a**. A mean efficiency of 90% and a maximum efficiency of 98% can be realized by the AAE design, which is superior compared to other methods. The absorption/emissivity spectra of the best designs also validate the optimization performance regarding uniformity and efficiency. Moreover, the AAE+VGGnet method only takes 2 minutes to generate 100 highly efficient designs with efficiency higher than 80%, while the computation time of direct TO and AAE + TO are around 164 hours and 64 hours, respectively. Here, TO serves two purposes: first, it is used to enhance the training set's quality and the NN's performance in the first phase; second, it aids in post-processing to ensure that the design is reliable and realistic. Subsequently, the same group reported that by connecting the AAE network with a differential evolution optimizer, the multi-parametric global optimization can be performed in the compressed design space, giving rise to a greatly enhanced optimization search efficiency [32].

Apart from using TO to enhance the performance of NNs, adjoint method, which is the backbone acceleration strategy for TO, can also be blended with NNs to help to retrieve the gradient information of NNs by

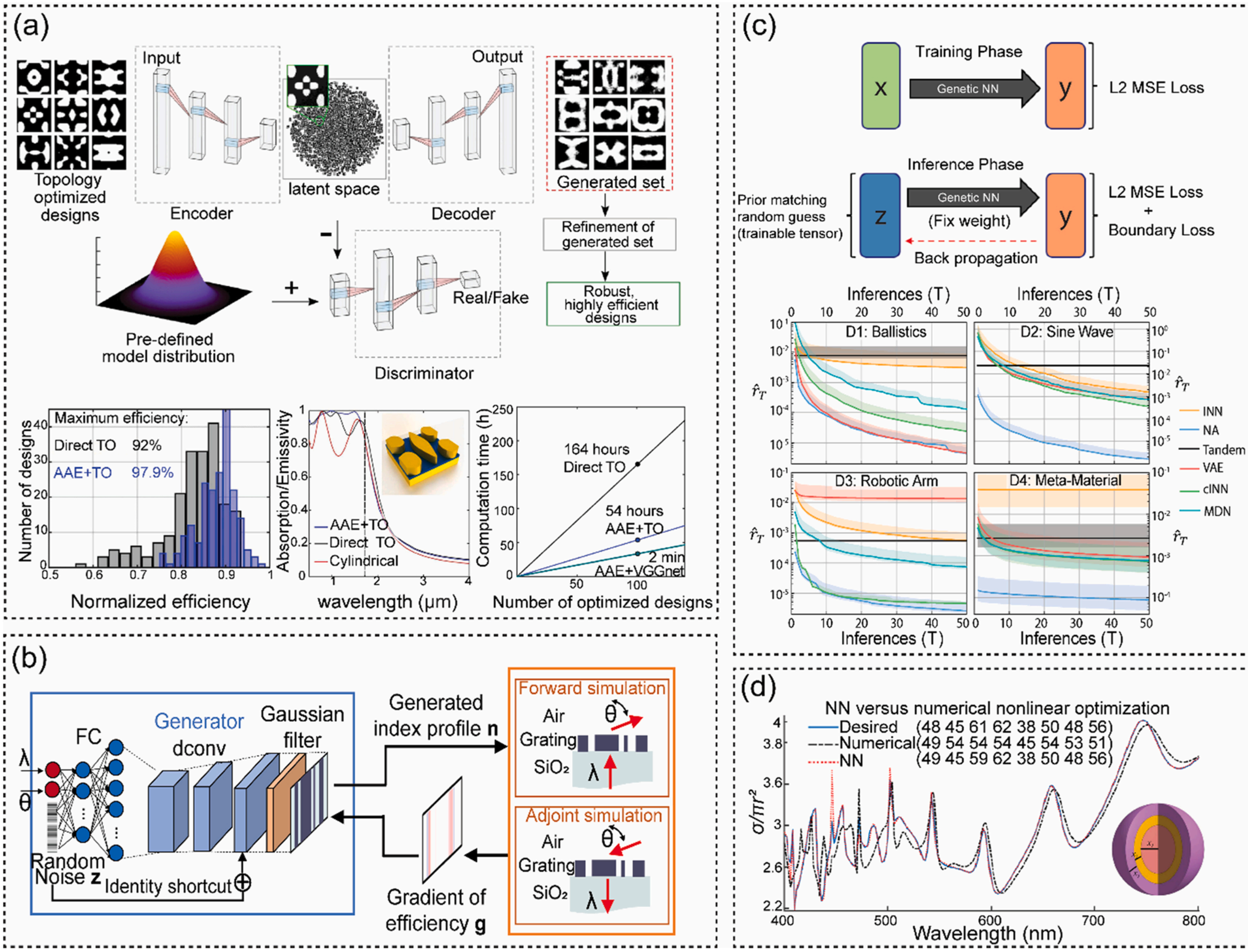

Fig. 2. Fusing topology optimization and adjoint method with neural networks. (a) Top: Workflow of AAE-assisted topology optimization for thermal emitter design. Bottom: Normalized efficiency, absorption/emissivity, and the computation time of the thermal emitters designed by different methods. (b) Schematic of GLOnet for metagrating design, where the gradient solving process is replaced by the adjoint method simulation. (c) A neural-adjoint method for universal inverse design tasks. Top: Illustration of the forward model training process and the inverse design by the backpropagation of NNs. Bottom: Comparison of the performance of 6 models for 4 different situations. (d) Comparison between the target function, numerical results, and inversed design prediction of the scattering cross-section of a multi-layer nanoparticle.

(a) is reproduced from Ref. [31] with permission; (b) is reproduced from Ref. [33] with permission; (c) is reproduced from Ref. [35] for permission; (d) is reproduced from Ref. [36] with permission.

employing one forward and one adjoint simulation. Recently, J Jiang et al. proposed an interesting approach to integrating the adjoint method with NNs for optimizing diffractive metagratings [33]. Prior to this work, the same group already demonstrated that the adjoint method can help with the TO of metasurfaces to deflect light at large angles with high efficiencies [25]. In this paper, they further improve the performance of the metagrating with global topology optimization networks (GLOnets), which are constructed by incorporating the adjoint method with generative optimization networks. As shown in Fig. 2**b**, the deflection angle θ, wavelength λ, and random noise vector z are fed into the NNs as input and then processed by the fully connected layers and the deconvolution layers. After applying a Gaussian filter to ensure that the generated pattern meets the minimum feature size for fabrication, metagratings with certain refractive index distributions within the design area are generated. Different from the conventional NNs, in which the objective function can be directly calculated, this physics-driven approach uses forward and adjoint simulations for a batch of structures to obtain gradient descent information of the objective function. Then the gradient will be averaged and back-propagated to update the weights of neurons. The training process in GLOnet is essentially identical as the iteration in conventional adjoint algorithms by applying the chain rule again, so that the gradient can be further backpropagated to the network parameters. By iteratively updating the parameters of the NNs, the diffraction efficiency at the desired angle and wavelength is optimized. The authors have made a comparison between the GLOnet and the adjoint method, confirming that the NNs show better or similar results compared to the conventional approach. More specifically, 500 devices are designed and optimized for each wavelength and angle pair using GLOnet and adjoint-based TO, and it turns out that 75% of the devices from the conditional GLOnet have efficiencies higher than those from adjoint-based optimization. As a result, the GLOnet, once trained, can perform inverse design more efficiently compared to conventional TO. Additionally, using the traditional adjoint method, the inverse design process must be repeated whenever the target function, such as the required deflection angle or working wavelength, is modified for new tasks. Retraining the GLOnet model, however, is not required for distinct target functions at different wavelengths or deflection angles.

For the inverse design with the aid of NNs, the Tandem model [10] and invertible NNs [34] have shown their potential to avoid the one-to-many mapping problem and provide an effective solution for the target objective function. Inspired by the conventional adjoint method, S. Ren has proposed a neural-adjoint method [35] and proven that for various benchmark activities, this straightforward strategy can yield the most accurate results in comparison to other approaches in several specific tasks. As shown in Fig. 2**c**, the workflow of the neural-adjoint method consists of two steps. First, a forward NNs to evaluate $y = f(x)$, which connects the design and the optical response y, is constructed and trained in a conventional manner by a pair of input and output dataset. Then for a user-define target, a loss function $\mathscr{L}$ is defined between predicted $(\hat{y})$ and true (y) responses. The gradient $\partial\mathscr{L}/\partial x$ is used to implement descent towards locally optimal x values similar to other classical optimization algorithms. With the help of NNs built in the first step, a closed-form differentiable expression for the simulator can be obtained, which can simplify the process of gradient descent. Furthermore, the additional term for the loss function called boundary loss, is considered in the neural-adjoint method to increase the likelihood that solutions would be created inside the training data domain, resulting in more accurate solutions when evaluated by the simulator. Compared to other models, the neural-adjoint method shows the lowest error among all models, tasks, and the number of samples that are considered, since it can search the whole x-space and precisely localize inverse solutions. However, the disadvantage of the neural-adjoint method also exists: it may easily reach a poor local minimum for complex design problems. Therefore, a good initial design that is close enough to the global minimum will be beneficial. There are a few published papers that use a similar method to solve specific inverse design problems. For example, as shown in Fig. 2**d**, J. Peurifoy et al. have reported that the light scattering of the multilayer nanoparticles can be optimized by NNs [36]. For the forward model, the input parameters of the NNs are the thickness of each layer with fixed materials and the output is the spectrum information. 50,000 examples are generated from the transfer matrix method for the training dataset and a fully connected network with four layers and 250 neurons per layer is trained with those data. First, they verify that their NNs can accurately predict the spectrum of the test structural parameters referring to the sharp peaks and high quality factors. Then, they run the NNs "backward" by using the analytical gradient for inverse design applications. Finally, the authors compare the NN-aided inverse design and other numerical nonlinear optimization methods, and find their approach has better performance with respect to the accuracy of the reconstructed spectrum. Moreover, compared to the full-wave simulation, the running speed for the inverse design process has been accelerated more than 100 times.

3. Integrating evolutionary algorithm with neural networks

An evolutionary algorithm (EA) is a metaheuristic algorithm based on generic population [37,38]. With the ability to efficiently solve global optimization problems by mimicking the processes of selection, reproduction, mutation, and crossover in nature, it has become one of the most popular inverse design methods for integrated photonics and planar optics [39–42]. Using this method, researchers have successfully demonstrated waveguide couplers [43], waveguide routers [44], waveguide reflectors [45], broadband and full-color meta-holograms [46], and wavefront shaping [47]. In the following, we will focus on GA, a typical EA, as the example. The workflow of GA mainly involves four steps: First, the initial population is generated randomly, containing a certain number of chromosomes with genes that denotes the input variables. Then, the fitness score, a numerical indicator of how well a proposed solution fits the requirement, is calculated for the parents. The finest individuals will be chosen using a selection procedure based on a roulette wheel and the fitness score. In the next step, the individuals inside the population exchange the genes of parents to reproduce offspring. Finally, after adding the offspring to the population, random mutation is executed so that the population is gradually evolved towards the optimized solution. This four-step process normally repeats several times before the termination requirement is met. Despite the fact that GA has been used extensively for inverse design over the past decades, only until recently have people proposed to combine GA with NNs to improve the performance of the photonic design [48–50]. We will discuss various integration strategies for GA and NNs for different objectives in this section. For example, GA can assist in configuring the hyperparameters of NNs or choosing the meta-atoms for the supercell. On the other hand, NNs can also be combined with traditional GA to significantly improve its performance and operation speed.

In 2019, T. Zhang et al. proposed to use the GA to design the network architecture and select the hyperparameters for NNs [51], as shown in the top panel of Fig. 3**a**. As a result, precise spectrum prediction and inverse design of plasmonic waveguides can be realized by the optimized NNs. The hyperparameters of a neural network, including the number of layers, neurons per layer, the optimizer for weights, and the activation functions at the end of each layer, determine the final performance of the neural networks. However, in the conventional model building process, the setting of the network is always based on prior experience or laborious commissioning. In contrast, in this work, the four hyperparameters are set as the variables of GA to optimize the performance of network architecture, which can be indicated by the fitness scores of different generations. After it reaches a high value, the prediction accuracy, convergence, and calculation time can be improved. For spectrum prediction, the structural parameters including the length, width and gap distance of the cavities are fed into the NNs to obtain the transmission response of a plasmonic waveguide. The fitness scores of three structures THRC, FORC and FIRC, which stands for three, four and five rectangular cavities, show that the accuracy of the models can be iteratively improved (bottom left panel of Fig. 3**a**). The transmission spectra predicted by the optimized NNs can perfectly match the FDTD simulation result (bottom right panel of Fig. 3**a**).

Another interesting topic that can benefit from introducing EA to NNs is the design and optimization of complex metasurfaces [50,52,53]. As shown in the top panel of Fig. 3**b**, Z. Liu and co-workers present a hybrid framework that combines a compositional pattern-producing network (CPPN) and cooperative coevolution (CC) to deal with the inverse design problem of metamolecules composed of multiple meta-atoms with complex topologies [52]. The target function of this metasurface design is polarization conversion and anomalous wave deflection. The CPPN, which is widely used as the generator of the generative network, can decode a batch of latent vectors including x_i, y_i, r_i and a bias vector v to candidate patterns consisting of s_i at each pixel. Then CC is utilized to retrieve a set of vectors v in the latent space that can meet the target functions, specifically, the output polarization state, intensity, and phase distribution. To shorten the running time of the model, the authors execute the full-wave simulations of 8000 meta-atoms with various shapes and use the results to train a neural network simulator. In the end, by integrating two meta-atoms inside one metamolecule selected by the CC method as shown in the bottom panels of Fig. 3**b**, the authors verify the polarization conversion from 0° to 30° and 45° with linearly polarized incidence. They also implement the design of a metasurface, in which the supercell has eight meta-atoms. The metasurface can convert left circularly polarized light to its cross-polarization (i.e., right circularly polarized light), and deflect the cross-polarized light to a specific angle. Very recently, the same group has published another paper that combines NNs with an EA-based optimizer to design cascading layers of metasurfaces with multifunctional capabilities [53]. The total response of the multilayer supercell is calculated by the matrix-chain multiplication of the wave matrix and optimized by an EA optimizer. Complex functions are achieved, including a polarization-multiplexed dual-functional beam generator, a second-order differentiator for all-optical computing, and a space-polarization-wavelength multiplexed hologram.

Thanks to its ability to significantly speed up the calculation for the optical responses of unknown devices, pre-trained NNs can replace the

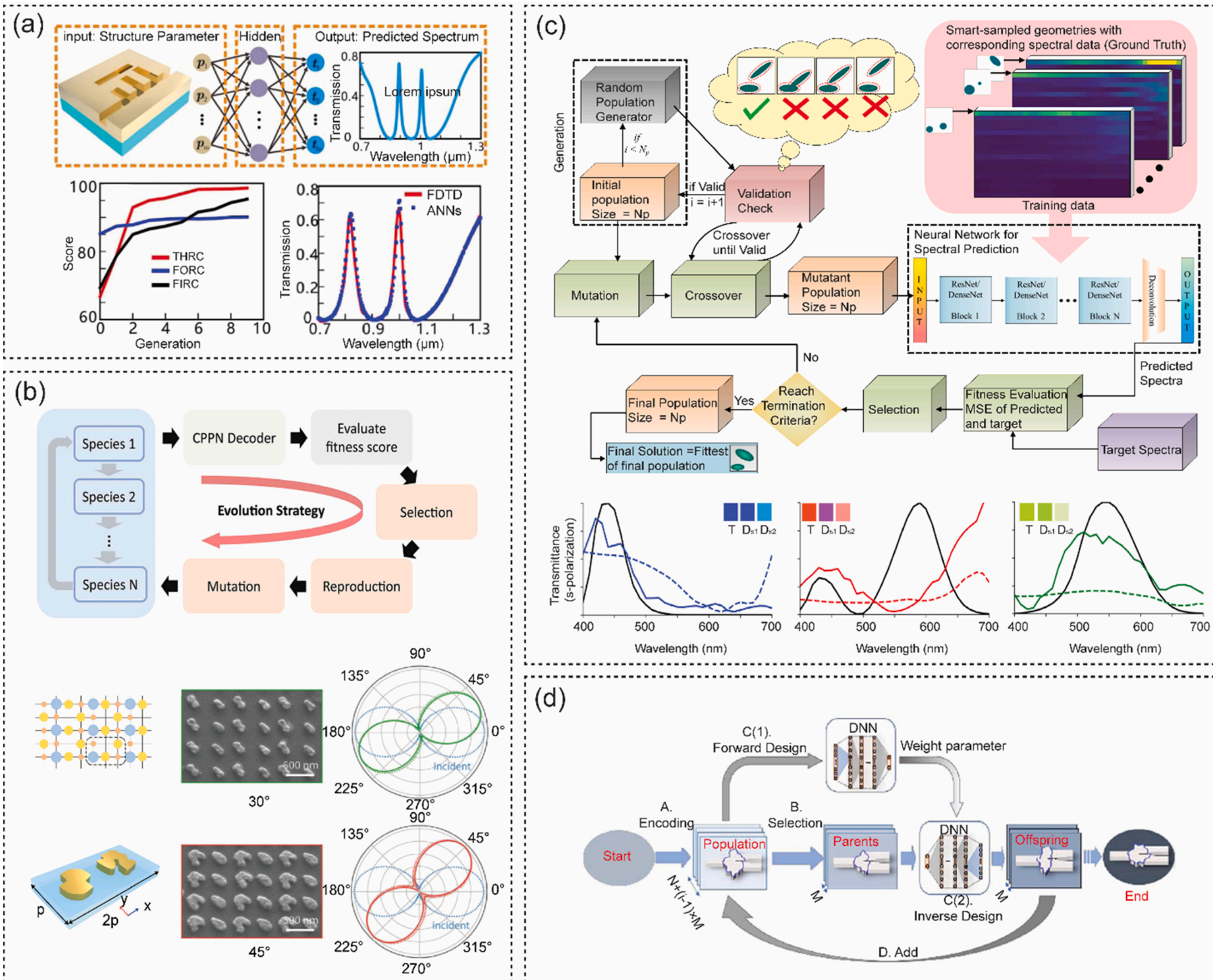

Fig. 3. Integrating evolutionary algorithm with neural networks. (a) Top: Illustration of the model framework for plasmonic waveguide design. Bottom: The fitness scores of three models for different generations, and the respective transmission spectra from FDTD simulation and NNs. (b) Top: Schematic of a hybrid model for metamolecules design. Bottom left: Schematic of the metamolecules' structure. Bottom middle and bottom right: Scanning electron microscope image of the fabricated samples and the measurement results for converting the incident polarization direction from 0° to 30° and 45°. (c) Top: Illustration of the surrogate-assisted evolutionary optimization method. Bottom: Simulation results for RGB color splitters. (d) Illustration for inverse design of on-chip beam splitters enabled by GA-based deep neural networks.
(a) is reproduced from Ref. [51] with permission (b) is reproduced from Ref. [52] with permission; (c) is reproduced from Ref. [54] with permission; (d) is reproduced from Ref. [55] with permission.

electromagnetic solver in the traditional inverse design method to accelerate the evaluation of candidate structures. Moreover, for the structure that can be characterized by a smaller number of structural parameters, the hybrid model can be further simplified. For instance, S. S. Panda and R. S. Hegde reported a surrogate-assisted evolutionary optimization method for the inverse design of metagratings with the functions of spectral filters and color splitters [54], as shown in Fig. 3**c**. Different from other works, the main framework in this model is the EA while the NN serves as the electromagnetic solver to evaluate the performance of the individuals in the population. The extended unit cell of the metagrating consists of several elliptical nanopillars without spatial overlapping, and then a model based on the framework of differential evolution optimization is built to search the full geometrical parameter space. Different from the conventional EA, the electromagnetic solver that can evaluate the loss function of each design inside the population is replaced by a pre-trained NN model to greatly accelerate the numerical optimization process. The authors have also discussed how the sampling method of parameter space and different feedforward architecture affect the final performance. Finally, they demonstrate three inverse design examples including polarization-insensitive RGB color filter, polarization-dependent RGB color filters, and RGB color splitters as shown in the bottom panel of Fig. 3**c**. Compared to feedforward architecture trained with randomly selected samples, deep neural network (DNN) architecture trained with k-means clustering strategy shows better performance regarding the fitness of the target spectrum and color purity in most cases.

For all the aforementioned hybrid frameworks, a large amount of data generated from the electromagnetic simulation are always required to train the NNs. Recently, Y. Ren have proposed a more flexible GA-based deep neural network method that only needs less than 3000 simulation data for the training process, an order of magnitude fewer than the previous works [55]. The basic workflow is presented in Fig. 3**d**. First, the initial polar vectors that describe the boundary of the optimization area and their numerical simulation results are encoded as population. The initial population plays two roles here: to generate the weight parameters in the DNN model for both forward and inverse design, and to be selected as parents for the following process according to their objective function. Since the crossover and mutation operations are replaced by the inverse DNN model, the devices' figure of merit data are set as input for the inverse DNN to produce offspring designs correlated to the parents. The new data are sent to the population and update the weight of DNN. This iteration is repeated several times until the termination requirements are satisfied. Several applications, including power splitters with different energy ratios and mode converters, were successfully demonstrated. The authors also proved that compared to the conventional GAN method, their GA-based deep neural network can have more comparable results but with a much smaller training dataset.

4. Combining Bayesian Algorithm and Gerchberg–Saxton algorithm with neural networks

In addition to the conventional optimization methods, some other strategies, such as Bayesian optimization (BO) [56,57] and Gerchberg–Saxton (GS) algorithm [58], have been used to assist the photonic design. BO is one algorithm that works for global optimization of black-box problems, where only the input and output of the model are provided while the structure of the function is unknown. For a typical BO process, an initial set of candidate solutions are generated first, and then the next most possible solutions are generated from the given candidates by Gaussian process regression and acquisition functions. In another word, the method will suggest the candidate that is most likely to have a globally optimized figure of merit. Utilizing all the information from previously searched points, this method is more efficient than brute-force search or random search. Y. Li et al. have recently introduced a self-consisting framework called BoNet [59], which combines BO and convolutional neural network (CNN) for electric field prediction and also inverse design for optimized chiral responses. The geometric parameters that determine the shape of the nanostructure are connected with the far-field spectrum and near-field distribution by BoNet. As shown in Fig. 4**a**, considering the required dimension for these two kinds of optical response, the dense layer and convolution layer are applied for the spectrum prediction and near-field distribution, respectively. Then, BO is iteratively applied to enhance the CNN model after training. Since it is hard to precisely predict for the parameters that have very different response compared to the parameters used to train the CNN, the authors utilize BO to improve the prediction accuracy for the target functions. To be more specific, BO can recommend new parameters with a better optical response. However, the CNN may not correctly evaluate these new parameters. The discrepancy is described by the error of the response obtained from the CNN prediction and FDTD simulation, respectively. If a large error occurs, it means that the features of the new designs (and their neighbors in parameter space) are not fully extracted by the CNN, so these data points can be further added to the training dataset to reinforce the model and improve the prediction accuracy. The far-field circular dichroism optimization at different wavelengths and a theoretical circular dichroism of up to 82% are confirmed by experiment. Moreover, since the BoNet can also accurately predict the near-field distribution, the intrinsic physics for the origin of optical chirality can be revealed. The electric-field distribution from cathodoluminescence spectroscopy and measured reflection spectra match well with the prediction.

The GS algorithm [58] is one widely used phase-retrieval algorithm to calculate the phase profiles with designated intensity distribution at the input plane that can generate the desired holographic images at the far field. It iteratively replaces the amplitude at the image and far-field

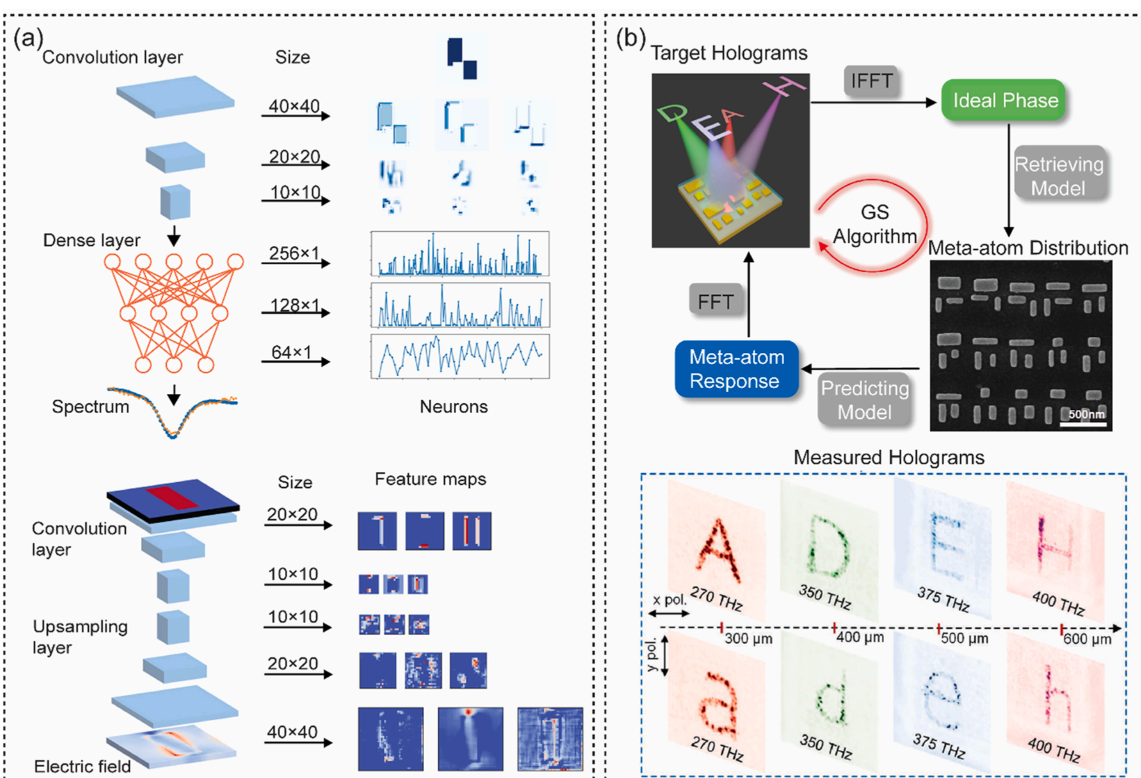

Fig. 4. Applying Bayesian algorithm and Gerchberg–Saxton algorithm with neural networks for inverse design. (a) Top: Schematic of BoNet for spectrum predication using dense layers. Bottom: Schematic of BoNet for near-field prediction using convolution layers and the corresponding feature maps from each layer. (b) Top: Schematic of the hybrid model for multi-functional metasurfaces holograms. Bottom: Experiment results of holograms under different combined illumination conditions of four frequencies and two polarizations.
(a) is reproduced from Ref. [59] with permission; (b) is reproduced from Ref. [60] with permission.

planes while keeping the calculated phase profiles after Fresnel diffraction or fast Fourier transformation. Recently, W. Ma and co-workers have integrated this non-gradient iterative optimization algorithm with NNs to realize multi-functional metasurfaces holograms that can generate distinct holographic images for different incidence conditions [60]. The designed unit cell is composed of three nanodisks, which can be described by nine structural parameters, including the widths and lengths of nanodisks and the gaps between them. The developed NNs consist of a forward model, which predicts the complex reflection spectrum from the given structure, and an inverse design model to retrieve the metasurface design for the desired reflection spectrum response. As shown in the top panel of Fig. 4**b**, the NNs are coupled with the GS algorithm to form an end-to-end design loop. First, the model retrieves the structure from the phase requirement. Then, instead of using the ideal phase value at the metasurfaces plane, the authors use the actual optical response calculated by the forward model to generate the holographic images at the far field. By considering the real but not necessarily the ideal phase response at the metasurfaces plane during the iterative GS algorithm, the generated holograms could show better qualities than those designed by the conventional GS method when various incidence wavelengths and polarizations are involved. As shown at the bottom of Fig. 4**b**, up to 8 different holographic images with different illumination conditions are experimentally demonstrated, in very good agreement with the simulation results. Moreover, the authors have demonstrated multi-functional focusing lenses by integrating gradient-based optimization with NNs.

5. Conclusion

In this mini-review, we briefly introduce the working principles of the classical inverse design approaches, including the evolutionary algorithm and the topology optimization enabled by the adjoint method. Then we comprehensively discuss how to combine the conventional inverse design approaches and some other optimization methods with the NNs to further boost the flexibility, efficiency, and capability of the models. From the highlighted works discussed in this review, we can recognize that the hybrid inverse design models show unique features inherited from both the NNs and optimization methods. We can flexibly combine optimization techniques with NNs based on the target functions, enabling both tools to perform to their full potential. On one hand, the commonly used optimization methods can be utilized to further optimize the configuration and hyperparameters of NNs, which are usually important but defined manually in NNs. Additionally, some discrete variables, such as material choice and category of geometries, cannot be directly updated by gradient-based NNs alone. In contrast, this task is not an issue for non-gradient-based optimization methods like GA. The full-wave simulation and geometry creation, on the other hand, take the majority of the computing time during the optimization process. However, NNs could be used as extremely fast and accurate electromagnetic solvers or design generators once they are well trained. To make sure that the readers can clearly understand the various hybrid models and get inspired to adopt some of the methods for their own studies, in Table 1 we have summarized the framework of the hybrid models, the specific applications, the working principles and the advantages of the representative works.

We believe that more real-world applications with on-demand sophisticated field manipulation, high efficiency, and achievable fabrication features will be realized by the advanced algorithms combining optimization methods and artificial intelligence, which own increasing flexibility and improved performance. We anticipate that as the inverse design methodologies further develop and become more practical, more powerful applications, such as multi-functional metasurfaces, all-optical neural networks, and on-chip optical computing units will emerge. Complicated optical field manipulation, low energy consumption, and feasible fabrication features are essential for this vision, and these aspects need to be considered during the design process. In the near future, the hybrid inverse design approaches detailed in this mini-review will make the procedure easier and propel optical design to an unprecedented level.

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.

Table 1
Comparison of different hybrid models for photonic design.

Hybrid models	Specific methods/ networks	Applications	Working principles and advantages	Reference
NN+TO/ Adjoint method	AAE+VGGnet	Thermal emitters	Applying the TO to improve the quality of the training data, the performance of the NN after the training, as well as the postprocessing so that the designs are robust and realistic.	**Ref.**31,32
	GLOnets	Diffractive metagratings	Optimizing the NN by the adjoint method. While the traditional adjoint technique can only be used for a limited number of tasks, the trained NN can be used for other tasks of the same type.	**Ref.**33
	Neural-adjoint method	Metamaterials; Multilayer nanoparticles	Using the adjoint method and the backpropagation of the trained surrogate model to perform an accurate inverse design. No need to train additional NN including generative model or inverse model.	**Ref.**35,36
NN+GA	/	Plasmonic waveguides	Optimizing the hyperparameters via GA, instead of manual setting based on prior experience or laborious commissioning.	**Ref.**51
	CPPN + CC	Polarization converters and multi-channel metasurfaces	The optimization of metasurfaces with complex functions is realized by NN decoding variables from latent space to the candidate structure and GA selecting the meta-atoms for the supercells.	**Ref.**52,53
	/	RGB color filters and splitters	Replacing the GA's electromagnetic solver with a pre-trained NN, which can significantly speed up the inverse design process.	**Ref.**54
	/	Power splitters; Mode converters	Replacing the crossover and mutation process of GA by the inverse DNN model, so that it can have similar results but with a much smaller training dataset compared to the GAN method.	**Ref.**55
NN+BO/GS	BoNet	Near-field and spectrum prediction	Appling BO to improve the prediction accuracy for the target functions, and then a better training dataset is recommended to the training dataset to reinforce the model and improve the prediction.	**Ref.**59
	NN + GS	Multi-channel holograms	Using the real phase response retrieved by the NN during the iterative GS algorithm, the generated multi-channel holographic images own better qualities than the conventional design.	**Ref.**60

Data availability

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

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References

[1] Y. LeCun, Y. Bengio, G. Hinton, Deep learning, Nature 521 (7553) (2015) 436–444.
[2] D. Silver, A. Huang, C.J. Maddison, A. Guez, L. Sifre, G. Van Den Driessche, J. Schrittwieser, I. Antonoglou, V. Panneershelvam, M. Lanctot, Mastering the game of Go with deep neural networks and tree search, Nature 529 (7587) (2016) 484–489.
[3] Y. LeCun, Y. Bengio, Convolutional networks for images, speech, and time series. The handbook of brain theory and neural networks, MIT Press, 1995.
[4] A.K. Jain, J. Mao, K.M. Mohiuddin, Artificial neural networks: a tutorial, Computer 29 (3) (1996) 31–44.
[5] W. Ma, Z. Liu, Z.A. Kudyshev, A. Boltasseva, W. Cai, Y. Liu, Deep learning for the design of photonic structures, Nat. Photonics 15 (2) (2021) 77–90.
[6] Y. Xu, X. Zhang, Y. Fu, Y. Liu, Interfacing photonics with artificial intelligence: an innovative design strategy for photonic structures and devices based on artificial neural networks, Photonics Res. 9 (4) (2021) B135–B152.
[7] R.S. Hegde, Deep learning: a new tool for photonic nanostructure design, Nanoscale Adv. 2 (3) (2020) 1007–1023.
[8] Z. Liu, D. Zhu, L. Raju, W. Cai, Tackling photonic inverse design with machine learning, Adv. Sci. 8 (5) (2021) 2002923.
[9] P.R. Wiecha, A. Arbouet, C. Girard, O.L. Muskens, Deep learning in nano-photonics: inverse design and beyond, Photonics Res. 9 (5) (2021) B182–B200.
[10] D. Liu, Y. Tan, E. Khoram, Z. Yu, Training deep neural networks for the inverse design of nanophotonic structures, ACS Photonics 5 (4) (2018) 1365–1369.
[11] I. Malkiel, M. Mrejen, A. Nagler, U. Arieli, L. Wolf, H. Suchowski, Plasmonic nanostructure design and characterization via deep learning, Light Sci. Appl. 7 (1) (2018) 1–8.
[12] S. So, J. Mun, J. Rho, Simultaneous inverse design of materials and structures via deep learning: demonstration of dipole resonance engineering using core–shell nanoparticles, ACS Appl. Mater. Interfaces 11 (27) (2019) 24264–24268.
[13] Y. Chen, J. Zhu, Y. Xie, N. Feng, Q.H. Liu, Smart inverse design of graphene-based photonic metamaterials by an adaptive artificial neural network, Nanoscale 11 (19) (2019) 9749–9755.
[14] J. Yang, K. Cui, X. Cai, J. Xiong, H. Zhu, S. Rao, S. Xu, Y. Huang, F. Liu, X. Feng, Ultraspectral imaging based on metasurfaces with freeform shaped meta-atoms, Laser Photonics Rev. (2022) 2100663.
[15] W. Ma, F. Cheng, Y. Xu, Q. Wen, Y. Liu, Probabilistic representation and inverse design of metamaterials based on a deep generative model with semi-supervised learning strategy, Adv. Mater. 31 (35) (2019) 1901111.
[16] S.J. Wetzel, Unsupervised learning of phase transitions: from principal component analysis to variational autoencoders, Phys. Rev. E 96 (2) (2017), 022140.
[17] Q. Zhang, C. Liu, X. Wan, L. Zhang, S. Liu, Y. Yang, T.J. Cui, Machine-learning designs of anisotropic digital coding metasurfaces, Adv. Theory Simul. 2 (2) (2019) 1800132.
[18] J. Liu, D. Zhang, D. Yu, M. Ren, J. Xu, Machine learning powered ellipsometry, Light.: Sci. Appl. 10 (1) (2021) 1–7.
[19] S. So, Y. Yang, T. Lee, J. Rho, On-demand design of spectrally sensitive multiband absorbers using an artificial neural network, Photonics Res. 9 (4) (2021) B153–B158.
[20] W. Ma, F. Cheng, Y. Liu, Deep-learning-enabled on-demand design of chiral metamaterials, ACS Nano 12 (6) (2018) 6326–6334.
[21] P.R. Wiecha, O.L. Muskens, Deep learning meets nanophotonics: a generalized accurate predictor for near fields and far fields of arbitrary 3D nanostructures, Nano Lett. 20 (1) (2019) 329–338.
[22] H. Ren, W. Shao, Y. Li, F. Salim, M. Gu, Three-dimensional vectorial holography based on machine learning inverse design, Sci. Adv. 6 (16) (2020) eaaz4261.
[23] A.Y. Piggott, J. Lu, K.G. Lagoudakis, J. Petykiewicz, T.M. Babinec, J. Vučković, Inverse design and demonstration of a compact and broadband on-chip wavelength demultiplexer, Nat. Photonics 9 (6) (2015) 374–377.
[24] P.I. Borel, A. Harpøth, L.H. Frandsen, M. Kristensen, P. Shi, J.S. Jensen, O. Sigmund, Topology optimization and fabrication of photonic crystal structures, Opt. Express 12 (9) (2004) 1996–2001.
[25] D. Sell, J. Yang, S. Doshay, R. Yang, J.A. Fan, Large-angle, multifunctional metagratings based on freeform multimode geometries, Nano Lett. 17 (6) (2017) 3752–3757.
[26] Z. Lin, V. Liu, R. Pestourie, S.G. Johnson, Topology optimization of freeform large-area metasurfaces, Opt. Express 27 (11) (2019) 15765–15775.
[27] J.S. Jensen, O. Sigmund, Topology optimization for nano-photonics, Laser Photonics Rev. 5 (2) (2011) 308–321.
[28] T. Phan, D. Sell, E.W. Wang, S. Doshay, K. Edee, J. Yang, J.A. Fan, High-efficiency, large-area, topology-optimized metasurfaces, Light.: Sci. Appl. 8 (1) (2019) 1–9.
[29] F. Wang, J.S. Jensen, O. Sigmund, Robust topology optimization of photonic crystal waveguides with tailored dispersion properties, JOSA B 28 (3) (2011) 387–397.
[30] O. Yesilyurt, Z.A. Kudyshev, A. Boltasseva, V.M. Shalaev, A.V. Kildishev, Efficient topology-optimized couplers for on-chip single-photon sources, ACS Photonics 8 (10) (2021) 3061–3068.
[31] Z.A. Kudyshev, A.V. Kildishev, V.M. Shalaev, A. Boltasseva, Machine-learning-assisted metasurface design for high-efficiency thermal emitter optimization, Appl. Phys. Rev. 7 (2) (2020), 021407.
[32] Z.A. Kudyshev, A.V. Kildishev, V.M. Shalaev, A. Boltasseva, Machine learning–assisted global optimization of photonic devices, Nanophotonics 10 (1) (2021) 371–383.
[33] J. Jiang, J.A. Fan, Global optimization of dielectric metasurfaces using a physics-driven neural network, Nano Lett. 19 (8) (2019) 5366–5372.
[34] Kruse, J.; Ardizzone, L.; Rother, C.; Köthe, U., Benchmarking invertible architectures on inverse problems. arXiv preprint arXiv:2101.10763 2021.
[35] S. Ren, W. Padilla, J. Malof, Benchmarking deep inverse models over time, and the neural-adjoint method, Adv. Neural Inf. Process. Syst. 33 (2020) 38–48.
[36] J. Peurifoy, Y. Shen, L. Jing, Y. Yang, F. Cano-Renteria, B.G. DeLacy, J. D. Joannopoulos, M. Tegmark, M. Soljačić, Nanophotonic particle simulation and inverse design using artificial neural networks, Sci. Adv. 4 (6) (2018) eaar4206.
[37] Grefenstette, J.J. In *Genetic algorithms and machine learning*, Proceedings of the sixth annual conference on Computational learning theory, 1993; pp 3–4.
[38] J.H. Holland, Adaptation in natural and artificial systems: an introductory analysis with applications to biology, control, and artificial intelligence, MIT press, 1992.
[39] L. Shen, Z. Ye, S. He, Design of two-dimensional photonic crystals with large absolute band gaps using a genetic algorithm, Phys. Rev. B 68 (3) (2003), 035109.
[40] E. Kerrinckx, L. Bigot, M. Douay, Y. Quiquempois, Photonic crystal fiber design by means of a genetic algorithm, Opt. Express 12 (9) (2004) 1990–1995.
[41] G. Genty, L. Salmela, J.M. Dudley, D. Brunner, A. Kokhanovskiy, S. Kobtsev, S. K. Turitsyn, Machine learning and applications in ultrafast photonics, Nat. Photonics 15 (2) (2021) 91–101.
[42] L. Sanchis, A. Håkansson, D. López-Zanón, J. Bravo-Abad, J. Sánchez-Dehesa, Integrated optical devices design by genetic algorithm, Appl. Phys. Lett. 84 (22) (2004) 4460–4462.
[43] M.M. Spuhler, B.J. Offrein, G.-L. Bona, R. Germann, I. Massarek, D. Erni, A very short planar silica spot-size converter using a nonperiodic segmented waveguide, J. Light. Technol. 16 (9) (1998) 1680–1685.
[44] Z. Liu, X. Liu, Z. Xiao, C. Lu, H.-Q. Wang, Y. Wu, X. Hu, Y.-C. Liu, H. Zhang, X. Zhang, Integrated nanophotonic wavelength router based on an intelligent algorithm, Optica 6 (10) (2019) 1367–1373.
[45] Z. Yu, H. Cui, X. Sun, Genetically optimized on-chip wideband ultracompact reflectors and Fabry–Perot cavities, Photonics Res. 5 (6) (2017) B15–B19.
[46] Z. Jin, S. Mei, S. Chen, Y. Li, C. Zhang, Y. He, X. Yu, C. Yu, J.K. Yang, B. Luk'yanchuk, Complex inverse design of meta-optics by segmented hierarchical evolutionary algorithm, ACS Nano 13 (1) (2019) 821–829.
[47] Q. Feng, F. Yang, X. Xu, B. Zhang, Y. Ding, Q. Liu, Multi-objective optimization genetic algorithm for multi-point light focusing in wavefront shaping, Opt. Express 27 (25) (2019) 36459–36473.
[48] T. Zhang, Q. Liu, Y. Dan, S. Yu, X. Han, J. Dai, K. Xu, Machine learning and evolutionary algorithm studies of graphene metamaterials for optimized plasmon-induced transparency, Opt. Express 28 (13) (2020) 18899–18916.
[49] J. Guimbao, L. Sanchis, L. Weituschat, J. Manuel Llorens, M. Song, J. Cardenas, P. Aitor Postigo, Numerical optimization of a nanophotonic cavity by machine learning for near-unity photon indistinguishability at room temperature, ACS Photonics 9 (6) (2022) 1926–1935.
[50] Z. Liu, L. Raju, D. Zhu, W. Cai, A hybrid strategy for the discovery and design of photonic structures, IEEE J. Emerg. Sel. Top. Circuits Syst. 10 (1) (2020) 126–135.
[51] T. Zhang, J. Wang, Q. Liu, J. Zhou, J. Dai, X. Han, Y. Zhou, K. Xu, Efficient spectrum prediction and inverse design for plasmonic waveguide systems based on artificial neural networks, Photonics Res. 7 (3) (2019) 368–380.
[52] Z. Liu, D. Zhu, K.T. Lee, A.S. Kim, L. Raju, W. Cai, Compounding meta-atoms into metamolecules with hybrid artificial intelligence techniques, Adv. Mater. 32 (6) (2020) 1904790.
[53] D. Zhu, Z. Liu, L. Raju, A.S. Kim, W. Cai, Building multifunctional metasystems via algorithmic construction, ACS Nano 15 (2) (2021) 2318–2326.
[54] S.S. Panda, R.S. Hegde, A learning based approach for designing extended unit cell metagratings, Nanophotonics 11 (2) (2022) 345–358.
[55] Y. Ren, L. Zhang, W. Wang, X. Wang, Y. Lei, Y. Xue, X. Sun, W. Zhang, Genetic-algorithm-based deep neural networks for highly efficient photonic device design, Photonics Res. 9 (6) (2021) B247–B252.
[56] R. Patel, K. Roy, J. Choi, K.J. Han, Generative design of electromagnetic structures through Bayesian learning, IEEE Trans. Magn. 54 (3) (2017) 1–4.
[57] A. Sakurai, K. Yada, T. Simomura, S. Ju, M. Kashiwagi, H. Okada, T. Nagao, K. Tsuda, J. Shiomi, Ultranarrow-band wavelength-selective thermal emission with aperiodic multilayered metamaterials designed by Bayesian optimization, ACS Cent. Sci. 5 (2) (2019) 319–326.
[58] Z. Zalevsky, D. Mendlovic, R.G. Dorsch, Gerchberg–Saxton algorithm applied in the fractional Fourier or the Fresnel domain, Opt. Lett. 21 (12) (1996) 842–844.
[59] Y. Li, Y. Xu, M. Jiang, B. Li, T. Han, C. Chi, F. Lin, B. Shen, X. Zhu, L. Lai, Self-learning perfect optical chirality via a deep neural network, Phys. Rev. Lett. 123 (21) (2019), 213902.
[60] W. Ma, Y. Xu, B. Xiong, L. Deng, R.-W. Peng, M. Wang, Y. Liu, Pushing the limits of functionality-multiplexing capability in metasurface design based on statistical machine learning, Adv. Mater. 34 (16) (2022), 2110022.