Forward prediction and inverse design of metasurface via deep neural network integrating multi-task deep learning with genetic algorithm

Ziyi Wan, Yiru Zong, Yuan Zhang, Peng Zhang, Shan Wu

Key Laboratory of Functional Materials and Devices for Informatics of Anhui Educational Institutions, School of Physics and Electronic Engineering, Fuyang Normal University, Fuyang 236037, China

E-mail addresses: zpzp@mail.ustc.edu.com (P. Zhang), swu@fynu.edu.cn (S. Wu)

ABSTRACT The traditional design of metasurface mainly relies on complex numerical calculation, which is not only time-consuming and laborious but also requires designers with high professional ability. With the rapid development of artificial intelligence, the deep learning method has blossomed into an effective way to realize rapid design of metasurface. Here, a deep learning architecture that combines multi-task learning neural network and genetic algorithm (MGDNN) is proposed to realize the forward and inverse mapping between the metasurface and its optical response. For a SiN disk arrays metasurface, the forward reflected spectra and inverse structure design are achieved, greatly improving the design accuracy and efficiency. The accuracy rate of forward prediction is 96.7%, and that of inverse on-demand design is 83.9%, overwhelming most of conventional deep neural network (CDNN) thus far. Our proposed method would enable fast and accurate design and optimization of various kinds of metasurfaces with different functionalities, and is expected to play a significant role in the design of future nanophotonics devices.

INDEX TERMS Metasurface, Deep learning, Forward design, Inverse design, Multi-task learning, Genetic algorithm.

I. INTRODUCTION

Metasurfaces are two-dimensional artificial composites composed of periodic or non-periodic arranged sub-wavelength unitcell (Liu et al., 2019; Zeng et al., 2023; Huang et al., 2022; Al-Nuaimi et al., 2019).

Compared with metamaterials, metasurfaces have the advantages of a compact profile, easy processing, and low loss, which have attracted much attention from researchers in recent years. The electromagnetic wave can be flexibly controlled through the design of metasurface structure (Arbabi et al., 2015; Wang et al., 2016; Chen et al., 2018), which in turn will lead to breakthroughs in the fields of beam control (Cong et al., 2018), superlens (Khorasaninejad et al., 2016; Arbabi et al., 2018), and optical cloaking (Ni et al., 2015). However, the design of metasurface typically requires numerical simulation based on Maxwell ' s equations to analyze their electromagnetic response under varying structural parameters. Although this method is accurate, the design process is time-consuming and computationally expensive, relying heavily on the experience and expertise of the designer. Therefore, establishing precise mappings between metasurface and their optical responses, while enabling rapid prediction of multifunctional performance metrics, has emerged as a critical frontier in photonic device design.

Deep learning (DL), as an essential branch of machine learning, uses the multilayer structure of artificial neural network (ANN) to learn the potential connections between input and output data automatically.

Through establishing mapping rules between input and output data using multiple weight matrices, DL technology can avoid the tedious work in exploring the complex physical relationship. As a result, DL has been applied in multiple fields, such as computer vision (Wu et al., 2017; Voulodimos et al., 2018), language translation (Ahammad et al., 2024), drug design (Gupta et al., 2021), and so on (Abbeel et al., 2010; Kussul et al., 2017; Muhammad et al., 2021; Fujiyoshi et al., 2019). In nanophotonics, DL has been trained to forward predict optical response and inverse design structure with higher efficiency and lower time

consumption. For example, a 4-layer deep neural network (DNN) has been developed for rapid and accurate forward prediction of the scattering spectra of multi-layer nanoparticles (Peurifoy et al., 2018). A rapid optical response prediction and parametric optimization for all-dielectric metasurface can be predicted based on a physics-inspired deeplearning method (Noureen et al., 2022). A tandem architecture based on DNN has been proposed to solve the problem of " non-uniqueness " in the inverse design of nanophotonic structures (Liu et al., 2018). Moreover, Results in Optics journal homep age: www.scien cedirect.co m/journal/re sults-in-opti cs Results in Optics 23 (2026) 100988 DNN method has been also proposed through inserting a sigmoid function between the input and the first hidden layer to accurately predict the phase and group delay of metasurface (Jiang et al., 2021).

The combination of DNN and genetic algorithm (GA) can significantly improve the design efficiency of meta-atoms, accurately predict the response of meta-atoms in milliseconds, and quickly find the optimal structural parameters (Zhang et al., 2024). Convolutional neural networks (CNNs) have been also used to design metasurfaces. A BoNet framework combining Bayesian optimization and deep CNNs algorithms has been developed to predict and optimize the electric field distributions and reflection spectra of the nanostructures (Li et al., 2019). Zhang et al. (Zhang et al., 2021) have used deep CNNs to achieve forward prediction and inverse design of three complex metasurfaces in the microwave range. Yan Teng et al. (Teng et al., 2023) have developed forward prediction and inverse design models for terahertz metasurface by combining deep CNNs and GA, resulting in significantly improved design efficiency and accuracy.

Conventional metasurface design typically falls into two categories: a forward process requiring manual modeling, parameter sweeping, and iterative optimization, and an inverse process that relies on heuristic algorithms and cannot guarantee global optima. In contrast, DL simplifies this workflow by establishing a direct, data-driven mapping between design objectives and structural parameters, thus significantly improves efficiency and reduces the designer's burden (Qiu et al., 2019) (Fig. 1). Thus, we propose a MGDNN framework integrating multi-task deep learning with genetic algorithm, harnessing the accelerated learning capability of multi-task architectures and the global search capacity of genetic algorithm to enable efficient and accurate forward prediction and inverse design of metasurface. Furthermore, to solve the mismatch problem between the inputs and outputs, multi-wavelength data are introduced into the trained dataset. Eventually, for a SiN disk arrays metasurface, both forward reflection spectrum prediction and inverse structural design are completed within milliseconds, with results showing agreement with simulations.

II. MODEL AND METHODS

In deep learning, the quality, quantity, and diversity of datasets are critical determinants of model performance, as high-quality datasets can directly enhance prediction accuracy and generalization capabilities.

Here, a SiN disk array with structural parameters of height h , diameter d and period P deposited on silicon dioxide substrate of thickness H is designed (Fig. 2). The dielectric constants of SiN and silicon dioxide are set as 4.21 and 2.25, respectively (Leng et al., 2021; Wu et al., 2010). A total of 6336 datasets with different structural parameters were calculated using the finite-difference time-domain method (FDTD). Before training, 336 sets of data were exclusively allocated as the test set for performance evaluation of the MGDNN, with explicit exclusion from the training process. The remaining data were divided into training and validation sets using an 8:2 ratio, following common practice in the field of deep learning. The training set is used to train the model and calculate the loss function, updating parameters such as weights and biases through backpropagation algorithms. The validation set is used to evaluate the performance of the model during training to adjust hyperparameters and avoid overfitting.

Each data sample consists of structural parameter (h , d , P , and H), frequency point (101), and corresponding reflectivity R . Due to the inconsistency in the numerical ranges and scales of the reflectance spectra, spectral points, and structural parameters, the accuracy of the based design front-loads effort by generating data and training a model to enable fast prediction. The inverse heuristic design automates the search for optimal solutions through iterative evaluation and population updates within a heuristic algorithm. model prediction may be reduced if these data are directly input into the network for training. Therefore, to eliminate the influence of different input scales on the generalization ability of the model, we adopted the Min-Max Normalization method (Patro and Sahu, 2015) to preprocess the spectral data and linearly map it into the (0, 1) range, so that the three parameters have the same metric, thus eliminating the numerical differences between different parameters, and improving the efficiency of the model training and the accuracy of the prediction.

The main purpose of establishing a forward neural network is to obtain the optical response of metasurface efficiently and accurately.

However, the input often consists of low-dimensional structural parameters, while the output is a high-dimensional optical property, such as a spectrum. There is an imbalance between the input and output dimensions, and due to the high nonlinearity of Maxwell's equations, a small number of input features may have difficulty fitting a large amount of output data better (Hegde, 2020). To this end, we introduce multi-wavelength data into the dataset to avoid

the problem of dimension mismatch between input and output data, enabling the model to learn the complex mapping relationship between structural parameters and optical properties more efficiently. Meanwhile, the neural network optimized by GA is more likely to converge to a better solution when solving complex nonlinear problems (Chiroma et al., 2017). Based on this, a MGDNN is proposed and encoded by PyTorch library. As is shown in Fig. 2a , the forward neural network consists of an input layer, shared hidden layers, task-specific output layers, and a final output layer.

The network's input is the 4 structural parameters, and 101 frequency points, which are combined into a 105-dimensional vector. The task-specific output layers contain 101 independent task layers, each with only 1 neuron, representing the reflectance r predicted by the model at this spectral point. The outputs of all task layers are spliced to the reflected spectrum R . It should be emphasized that the number of neurons in each layer of the shared hidden layer is obtained by GA optimization shown in Fig. 2b . The number of neurons in each layer is sequentially constituted as an array, which is regarded as the chromosome in the initial population. Firstly, 30 chromosomes are randomly generated to form the initial population, with crossover probability and mutation probability of 0.5 and 0.1, respectively. The population initialization model employs a roulette wheel selection method to choose the two best chromosomes in a population for genetic crossover.

After several population updates, the chromosome with the best fitness is obtained, and the designed model is updated with this chromosome.

After 300 iterations, the optimal number of neurons in each layer is 128, 256, 256, 16, and 16, respectively.

After fixing the random seeds and performing several simulation comparisons, we finally chose the Adam optimizer with a learning rate of 0.0005 to train the neural network. The batch size is set as 32, and the ReLU function is used as the activation function of the model. The combination of the exponential of absolute distance and the mean square error (MSE) is used as the loss function, as defined by:

$$[\text{Loss} = \frac{1}{N}\sum_{i=1}^{N} \exp\left(\left|\frac{R_{pred}}{R_{real}}\right|\right) + \frac{1}{N}\sum_{i=1}^{N} \frac{R_{pred}}{R_{real}}] \qquad (1)$$

By introducing an exponential term into MSE loss, the penalty for large errors is further enhanced, improving the performance of the model (Mall et al., 2020). properties. To achieve this, the target spectrum is parameterized into a vector form. However, a fundamental challenge in inverse design is the non-uniqueness of solutions, where vastly different structures can yield similar spectral responses.

To alleviate this problem, a deep neural network whose architecture is optimized by a genetic algorithm is employed (Fig. 3). The genetic algorithm optimizes the number of hidden layers and the number of neurons in each layer, with the verification set performance serving as the fitness criterion. The optimal network structure is five hidden layers, and the number of neurons in each layer is 128, 256, 256, 2048 and 128, respectively. Since the structure contains a large number of neurons, the study introduced a learning rate attenuation mechanism and dropout layer to prevent the model from overfitting. By feeding validation data to the network every 100 epochs to evaluate the model's performance and gradually reducing the learning rate, the model can converge more stably at the end of training, effectively reducing the risk of overfitting.

The network is trained with a hybrid loss function that combines the conventional parameter loss with a physics-informed.

This is calculated using a pre-trained, differentiable forward prediction network (see Table 1 for details) which acts as an embedded simulator. For any predicted set of structural parameters, this forward network generates the corresponding spectrum. The reconstruction loss then quantifies the discrepancy between this predicted spectrum and the original target spectrum. By prioritizing the physical accuracy of the output, this loss function guides the network to discover functional designs that correctly reproduce the target optical performance, rather than merely approximating a non-unique structural ground truth.

III. RESULTS

To prove the accuracy of the design method, several groups of data are randomly selected from the test set, and the prediction ability of the network is verified by comparing with the FDTD simulation and CDNN.

The layer sizes of CDNN are fixed to the best configuration discovered by GA in the single-task setting, ensuring identical capacity while isolating the contributions of MTL and GA. Results are shown in Fig. 4a - 4d , in which the blue line, red dash line, and dark blue dotted line represent the MGDNN, CDNN and simulated results. It is obvious that, compared with the CDNN method, the predicted results of the MGDNN method are in better agreement with the simulated results, indicating that the proposed model has better prediction ability for test set samples. Besides, neural network. After 3,000 iterations, training losses and validation losses are 0.00098 and 0.0021, respectively. The smooth decreasing trend and small loss values indicate that the network performed well during the training process.

To better estimate the performance of the model, the mean absolute error (MAE) is adopted as the error metric, which The error distribution of test set data is shown in Fig. 4f .

The average error of the MGDNN method is 0.0008, and the prediction accuracy rate is 96.7% (the accuracy rate is defined as the MAE between the predicted value and the actual value of the model). A performance comparison between the proposed MGDNN and other design methods is summarized in Table 2 . The results demonstrate that MGDNN not only improves efficiency but also maintains high prediction accuracy.

For the inverse design process, the on-demand design capability of MGDNN is verified by predicting metasurface structural parameters based on the target reflection spectrum. First, the target reflection spectrum data is preprocessed and input into the trained inverse network to obtain the predicted structural parameters. Then, these predicted structural parameters are input into the previously trained forward network to obtain the predicted reflection spectra. To further verify the accuracy of the prediction results, the FDTD simulation method was used to simulate the predicted structural parameters and obtain the corresponding simulation spectra. Finally, the target reflection spectrum, MGDNN and FDTD results of the predicted structure are compared to evaluate the prediction accuracy of inverse network.

In Fig. 5a , the red line, blue line, and dark blue dot line are the target, MGDNN and FDTD reflected spectrum of the predicted structure, respectively. Insets in Fig. 5a are the true and predicted structural parameters, in which it can be seen that the MGDNN model can identify the geometric parameters closest to the requirements as long as they are physically realizable (Fig. 5). To verify the superiority of genetic algorithm optimized network architecture, Fig. 5b – 5c shows the comparison of prediction results between the MGDNN and the CDNN in the form of a bar chart, in which it can be seen that the MGDNN significantly improves the prediction accuracy. A further evaluation using MAE gave an error of 0.003, corresponding to the MGDNN prediction accuracy of 83.9%. The MGDNN method not only improves the prediction ability of the network but also validates the effectiveness of genetic algorithm in deep learning model optimization.

The most significant advantage of deep learning-based approach is its computational efficiency. The MGDNN model completes the inverse design task in approximately 0.9256 s, marginally outperforming the CDNN model (0.97 s). This proves that MGDNN can efficiently and accurately achieve metasurface design.

IV. CONCLUSION

Inspired by deep learning, a MGDNN method integrating multi-task learning and genetic algorithm is proposed to efficiently and accurately achieve forward prediction and inverse design of metasurface. In the forward prediction, the MGDNN can accurately predict the metasurface reflection spectra from geometric parameters, with a prediction accuracy rate of 96.7%. In the inverse design, given the target spectrum, the prediction accuracy rate of MGDNN is 83.9%. These results demonstrate the ability of the MGDNN model to capture the complex nonlinear relationship between the physical structure and its optical response.

ACKNOWLEDGMENT

Thanks to its high accuracy and efficiency, our proposed MGDNN method is expected to play a significant role in the design of future nanophotonics devices and to have other advanced applications. It should be noted that, as with most data-driven approaches, the model's performance is contingent on the coverage of the training data, and its predictive capability is optimized for interpolation within the convex the test set,NOs.149, 1636, 2007, 2700). (e) The training loss and validation loss of the forward neural network. (f) Comparison of error calculation between the proposed method and the CDNN method test set. hull of the training distribution. For targets exhibiting fundamentally novel features far outside this distribution, performance may degrade.

REFERENCES

[1] Abbeel, P., Coates, A., Ng, A.Y., 2010. Autonomous helicopter aerobatics through apprenticeship learning. Int. J. Rob. Res. 29, 1608 – 1639.

[2] Ahammad, S.H., Kalangi, R.R., Nagendram, S., Inthiyaz, S., Priya, P.P., Faragallah, O.S., Mohammad, A., Eid, M.M.A., Rashed, A.N.Z., 2024. Improved neural machine translation using Natural Language Processing (NLP). Multimed. Tools Appl. 83, 39335 – 39348.

[3] Al-Nuaimi, M., He, Y., Hong, W., 2019. Design of inhonogeneous all-dielectric electromagnetic-wave diffusive reflectarraymetasurface. Antennas Wirel. Propag. Lett. 18, 732 – 736.

[4] Arbabi, E., Arbabi, A., Kamali, S.M., Horie, Y., Faraji-Dana, M., Faraon, A., 2018. MEMS-tunable dielectric metasurface lens. Nat. Commun. 9, 812.

[5] Arbabi, A., Horie, Y., Bagheri, M., Faraon, A., 2015. Dielectric metasurfaces for complete control of phase and polarization with subwavelength spatial resolution and high transmission. Nat. Nanotechnol. 10, 937 – 943.

[6] Chen, S., Li, Z., Zhang, Y., Cheng, H., Tian, J., 2018. Phase manipulation of electromagnetic waves with metasurfaces and its applications in nanophotonics. Adv. Opt. Mater. 6, 1800104.

[7] Chiroma, H., Noor, A.S.M., Abdulkareem, S., Abubakar, A.I., Hermawan, A., Qin, H., Hamza, M.F., Herawan, T., 2017. Neural networks optimization through genetic algorithm searches: a review. Appl. Math. Inf. Sci. 11, 1543 – 1564.

[8] Cong, L., Srivastava, Y.K., Zhang, H., Zhang, X., Han, J., Singh, R., 2018. All-optical active THz metasurfaces for ultrafast polarization switching and dynamic beam splitting. Light Sci. Appl. 7, 28.

[9] Fujiyoshi, H., Hirakawa, T., Yamashita, T., 2019. Deep learning based image recognition for autonomous driving. IATSS Res. 43, 244 – 252.

[10] Gupta, R., Srivastava, D., Sahu, M., Tiwari, S., Ambasta, R.K., Kumar, P., 2021. Artificial intelligence to deep learning: machine intelligence approach for drug discovery. Mol. Divers. 25, 1315 – 1360.

[11] Hegde, R.S., 2020. Deep learning: a new tool for photonic nanostructure design. Nanoscale Adv. 2, 1007 – 1023.

[12] Huang, Y.F., Jiang, Z.J., Liu, L., Zhang, H.C., 2022. Design of a 2-bit wide-angle coding metasurface for bistatic RCS reduction. Front. Mater. 9, 956061.

[13] Jiang, L., Li, X., Wu, Q., Wang, L., Gao, L., 2021. Neural network enabled metasurfacedesign for phase manipulation. Opt. Express 29, 2521 – 2528.

[14] Khorasaninejad, M., Chen, W.T., Devlin, R.C., Oh, J., Zhu, A.Y., Capasso, F., 2016. Metalenses at visible wavelengths: diffraction-limited focusing and subwavelength resolution imaging. Science 352, 1190 – 1194.

[15] Kussul, N., Lavreniuk, M., Skakun, S., Shelestov, A., 2017. Deep learning classification of land cover and crop types using remote sensing data. IEEE Geosci. Remote Sens. Lett. 14, 778 – 782.

[16] Leng, Q., Su, H., Liu, J., Zhou, L., Qin, K., Wang, Q., Fu, J., Wu, S., Zhang, X., 2021. Enhanced second-harmonic generation in monolayer MoS2 on suspended metallic nanostructures by plasmonic resonances. Nanophotonics 10, 1871 – 1877.

[17] Li, Y., Xu, Y., Jiang, M., Li, B., Han, T., Chi, C., Lin, F., Shen, B., Zhu, X., Lai, L., Fang, Z., 2019. Self-learning perfect optical chirality via a deep neural network. Phys. Rev. Lett. 123, 213902.

[18] Liu, D., Tan, Y., Khoram, E., Yu, Z., 2018. Training deep neural networks for the inverse design of nanophotonic structures. ACS Photonics 5, 1365 – 1369.

[19] Tretyakov, S.A., 2019. Intelligent metasurfaces with continuously tunable local surface impedance for multiple reconfigurable functions. Phys. Rev. Appl 11, 044024.

[20] Mall, A., Patil, A., Tamboli, D., Sethi, A., Kumar, A., 2020. Fast design of plasmonicmetasurfaces enabled by deep learning. J. Phys. D Appl. Phys. 53, 49LT01.

[21] Muhammad, K., Ullah, A., Lloret, J., DelSer, J., de Albuquerque, V.H.C., 2021. Deep learning for safe autonomous driving: current challenges and future directions. IEEE Trans. Intell. Transp. Syst. 22, 4316 – 4336.

[22] Ni, X., Wong, Z.J., Mrejen, M., Wang, Y., Zhang, X., 2015. An ultrathin invisibility skin cloak for visible light. Science 349, 1310 – 1314.

[23] Noureen, S., Mehmood, M.Q., Ali, M., Rehman, B., Zubair, M., Massoud, Y., 2022. A unique physics-inspired deep-learning-based platform introducing a generalized tool for rapid optical-response prediction and parametric-optimization for all-dielectric metasurfaces. Nanoscale 14, 16436 – 16449.

[24] Patro, S.G.K., Sahu, K.K., 2015. Normalization: A preprocessing stage. arXiv, 1503.06462.

[25] Peurifoy, J., Joannopoulos, J.D., Tegmark, M., Soljacic, M., 2018. Nanophotonic particle simulation and inverse design using artificial neural networks. Sci. Adv. 4, eaar4206.

[26] Qiu, T.S., Shi, X., Wang, J.F., Li, Y.F., Qu, S.B., Cheng, Q., Cui, T.J., Sui, S., 2019. Deep learning: a rapid and efficient route to automatic metasurface design. Adv. Sci. 6, 1900128.

[27] Teng, Y., Li, C., Li, S., Xiao, Y., Jiang, L., 2023. Efficient design method for terahertz broadband metasurface patterns via deep learning. Opt. Laser Technol. 160, 109058.

[28] Voulodimos, A., Doulamis, N., Doulamis, A., Protopapadakis, E., 2018. Deep learning for computer vision: a brief review. Comput. Intell. Neurosci., 7068349.

[29] Wang, W., 2016. Broadband metasurface holograms: toward complete phase and amplitude engineering. Sci. Rep. 6, 32867.

[30] Wu, Q., Liu, Y., Li, Q., Jin, S., Li, F., 2017. The application of deep learning in computer vision. Chinese Autom. Congr. (CAC) 2017, 6522 – 6527.

[31] Wu, S., Zhou, L., Wang, Y., Huang, C., Wang, Q., Wang, G., Zhu, Y., 2010. Phaselike resonance behavior in optical transmission of sandwich coaxial square ring arrays. Appl. Phys. Lett. 96, 253102.

[32] Zeng, B., Li, C., Cheng, H., Fang, B., Lu, J., Ma, X., Wang, L., Hong, Z., Jing, X., 2023. Anisotropic programmable metasurface beam splitter based on diode real-time control. Opt. Lasers Eng. 169, 107723.

[33] Zhang, M., Dong, P., Wang, Z., Hou, W., Wang, B., Yang, L., Li, K., Melikyan, V., 2024. Deep learning and genetic algorithm driven accelerated design for frequency-multiplexed complex-amplitude coding meta-hologram. Opt. Express 32, 38097 – 38111.

[34] Zhang, W., Xu, Y., Li, Z., Wu, S., Zhang, X., 2021. BoNet framework combining Bayesian optimization and deep CNNs algorithms for predicting and optimizing electric field distributions and reflection spectra of nanostructures. Nanophotonics 10, 1871 – 1877.