

Research on the Application of Artificial Neural Network Algorithm Model in Photonic Crystal Design

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Abstract—With the rapid development of today's communication field, the use of photonic crystals is more and more widespread. Since the mechanism of photonic crystals determines their optical properties, their application requires designers to design a lot of photonic crystal structures. This paper aims to introduce neural networks into the design of photonic crystal structures, so as to carry out the structure design of known photonic crystal bands. In the whole research process, the representative periodic structures of two-dimensional photonic crystals are selected to train the photonic crystal artificial neural network, and the backward prediction model from the target energy band to the structural parameters of the photonic crystal is further established. Finally, the prediction from the target band structure to the photonic crystal structure is realized. The results show that the neural network method can accurately learn the complex relationship between the photonic crystal structure and its optical properties, which provides a new technical approach for the rapid reverse design of photonic crystals.

Keywords—photonic crystal, artificial intelligence, neural network, backward prediction model

I. INTRODUCTION

As a kind of artificial electromagnetic medium, photonic crystals show broad application prospects in optical communication, optical integration and quantum optics due to their unique photonic bandgap characteristics. At present, most of the research on photonic crystals focuses on the structure study, and the optical frequency can be controlled by changing the structure of the photonic crystal. In this study, AI was used to predict the structure of photonic crystals. In this paper, based on a BP neural network, the mapping relationship between energy band characteristics and microcavity size is established for a two-dimensional photonic crystal microcavity structure, and the application potential of a neural network in the reverse design of photonic crystals is explored. The research contents include photonic crystal structure design and band calculation, sample data set preparation, BP neural network model construction, model training and performance evaluation, etc. Using the MPB software package to calculate the band map of two-dimensional photonic crystal and using the known band structure, a BP neural network was used to establish the nonlinear mapping relationship between band characteristics and microcavity size. By optimizing the network structure and training parameters, the effective prediction from the target band structure to microcavity size was realized, and the prediction result R^2 reached more than 0.999. It provides a new technical approach for fast reverse design of photonic crystals. Through this method, it can not only reduce a lot of time consumption required for simulation calculation, but also effectively avoid the problem that the global

convergence of reverse design is difficult.

II. LITERATURE REVIEW

For a long time, the design of various devices or systems has gone through three stages. When the mathematical theory has not been established, the new structure or design is usually assumed first, and then various experimental tests are carried out, which is the first stage. When a mathematical theory is established, the transition is to the second stage. In the second stage, new designs are iteratively tested by intuition or computation, but ultimately, the optimal solution cannot be found directly. In the third stage, when the generalized computational optimization method is introduced, the optimal performance is sought by establishing unconstrained or constrained problem models, and then the design scheme is obtained. This design method based on various optimizations in a broad sense is called reverse design [1]. The reverse design method in photonic devices and photonic systems refers to the algorithm of solving and discovering the corresponding optical structure based on the required functional characteristics [2]. Today, most reverse design is starting to use artificial intelligence, and compared with traditional optimization algorithms, data-driven design methods based on machine learning are rapidly emerging. Machine learning algorithms establish and extract models based on sample data, which is an important part of modern artificial intelligence [3]. At present, the research on machine learning mainly includes decision trees, random forests, Bayesian learning, support vector machines, artificial neural network and other aspects [4]. A decision tree is essentially to gradually build a decision tree model based on the available training set data, so that the model can correctly predict or classify the input [5]. Random forest is a method that enables the model to predict the corresponding output or classify the input data by integrating multiple regression trees or classification trees [6]. A Bayesian method algorithm is a kind of algorithm based on Bayes theorem [7]. The support vector machine (SVM) algorithm is a supervised learning model based on a statistical learning framework. Its implementation mechanism is to establish a hyperplane or a set of hyperplanes in high-dimensional or infinite-dimensional space, which can be used for regression or classification. The artificial neural network algorithm is essentially a way to simulate the thinking of the biological brain, which transforms the output of the previous level node into the output of the next level node in a hierarchical way. When a neural network involves a large number of network layers, it is called a deep learning model [8].

Photonic crystal is a kind of medium with periodic refractive index change, which can realize the control of the

reflection and transmission characteristics of light at a specific frequency. Through the design and manufacture of photonic crystals, it is possible to realize the control of light with a specific frequency, so as to realize the capture and control of tiny particles [9]. The reason is that defects in photonic crystals can act like filters, reflecting light at a fixed frequency. By introducing defects in the photonic crystal, local states can be formed in the band gap to realize the capture and manipulation of light with a specific frequency, which is of great value in ultra-small lasers, optical filters, and quantum information processing [10].

At present, the rapidly developing artificial neural network is a machine learning method that simulates the operation of biological neurons. By simulating the interaction of neurons, artificial neural network has shown excellent generalization ability and data fitting ability. Because a neural network can accurately construct the quantitative relationship between optical model and optical response, it has been widely used in the reverse design of optical devices. In recent years, artificial intelligence neural networks have been widely used in the field of optical research to establish predictions from the target energy band to the microcavity size through the input of its photonic crystal structure data. Most of the predecessors used a CNN neural network to predict the crystal structure. On the basis of the predecessors, this experiment used BP artificial intelligence neural network to predict the structural parameters of the photonic crystal. Because the BP neural network golden hook is relatively simple and does not have a large number of redundant connections, the convergence speed is faster, and the fitting degree is better in the case of small sample data. And its training speed is faster because the number of parameters is small.

III. EXPERIMENTAL DESIGN

A. Structure Design of Photonic Crystals

In this experiment, the two-dimensional dielectric cylindrical photonic crystal was designed, the background material was set as air, and the dielectric constant of the material was designed by using the “define” function, and the dielectric constant was set to $\varepsilon=12$. The period is 7 and the type of the lattice is the square lattice. Use the program (make cylinder (center 0 0) (radius 0.35) (height infinity) (material ss)) to design the constant medium cylinder radius is 0.35, and the height is infinite. The central microcavity is set at the origin (0,0), and the radius parameter is set to r . In the following, the lambda function is used to scan the radius r from 0 to 0.5, and the value of the radius parameter r is constantly changed to obtain multiple energy band images. On this basis, the k -space path is set up and the k points are designed to interpolate 10 points to calculate the number of energy bands to 50. The values of the photonic crystal structure design variables are presented in Table 1 below.

Table 1. Numerical table of photonic crystal design variables

Constant of permittivity	12	Number of k points	10
Conventional column radius	0.35	Number of energy bands	50
Radius of defect column	0-0.5	Supercell size	7x7

For the design of photonic crystals, two schemes were

used to design the experiment, and then the relationship between the prediction ability of photonic crystals and the electrolyte constant and other related parameters was explored, so as to change the structural parameters of photonic crystals and finally input them into MATLAB to obtain a better photonic crystal prediction neural network. The dielectric constant, period, interpolation number and the number of energy bands were modified in the experiment. Among the related parameters, the dielectric constant and the number of periods play the role of increasing the complexity of the photonic crystal and reducing the influence of the periodic boundary conditions and widening the band gap. The interpolation number of experimental parameters and the number of energy bands are modified to make the energy band curve smoother and obtain more high-frequency band information, but it will greatly prolong the calculation time. Its modified photonic crystal structure design variables are Table 2 below.

Table 2. Parameter table of photonic crystal control group

Constant of permittivity	15	Number of k points	20
Conventional column radius	0.35	Number of energy bands	100
Radius of defect column	0-0.5	Supercell size	9x9

The radius of the micro-cavity in the central medium will change with the continuous scanning of the lambda function, while the radius of the micro-cavity in the surrounding medium is 0.35, which will not change. The two media together form a crystal structure and form a specific energy band diagram, and the band gap can be determined according to the energy band diagram.

B. Neural Network Model Design

The MATLAB specific neural network consists of 491 samples and two hidden layers, in which the number of neurons in the hidden layer is 6 and 9 respectively. Among them, 400 samples out of 491 sample data are used as the training set to train the neural network, and 91 sample data are used as the test set to test the neural network.

The neural network training parameters are set to 10000 training rounds to seek higher prediction accuracy. The target error parameter is set to $1e-5$ in order to obtain more accurate fitting results. The specific program is `net.trainParam.epochs = 10000`; `net.trainParam.goal = 1e-5`; `net.trainParam.lr = 0.05`. Finally, the determination coefficient was calculated and the determination coefficient was observed as the evaluation standard of the fitting effect of the neural network.

IV. SAMPLE PREPARATION

MBP software package was used to design the photonic crystal structure and obtain the corresponding energy band. The dat file was output for subsequent detection and removal of NaN lines in the data using MATLAB, and the data in the dat file was read and cleaned to prepare for the training of artificial intelligence neural network. MATLAB was used to extract the energy band data, and the data were sampled by the parameters controlling the size of the microcavity. In this experimental program, the range of r was 0.01:0.001:0.5, a

total of 491 sample data were obtained. After extracting the data samples, the data were extracted and reorganized through the loop function, and the complete data set was constructed. Its specific data are shown in Table 3 below.

Table 3. Parameter table of photonic crystal dataset

Nk	0.1629	k	12x1 double
Nr	491	m	80
data	83x106 double	n	101
data_clean1	80x106 double	p1_dataset	1x491 double
inputdata	[]	r	1x491 double
inputdata1	[]	rowsAllNaN	83x1 logical
inputdata2	[]	te	12x55 double
inputdata3	80x101 double	w	12x50 double

MATLAB was used to extract the energy band information in the MPB file, the energy band information was plotted as the corresponding energy band diagram, and the photonic crystal band gap was analyzed according to the energy band diagram, as shown in Fig. 1 below. The specific band gap is between $0.22\omega a/2\pi c$ and $0.235\omega a/2\pi c$.

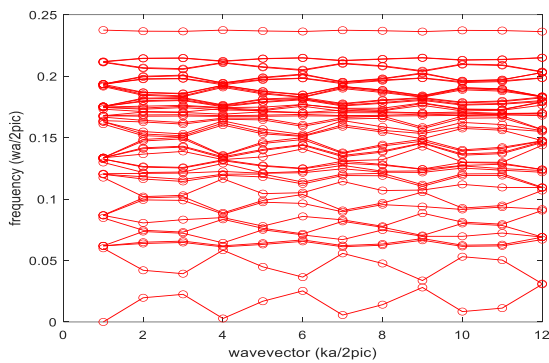


Fig. 1. Photonic crystal band diagram.

V. NETWORK MODEL TRAINING AND TESTING

The neural network program finally obtains the composition graph of the photonic crystal neural network from an input dimension to the hidden layer 1 composed of 9 neurons and then to the hidden layer 2 composed of 6 neurons. Finally, the one-dimensional results are output after processing by the output layer.

The number of training rounds is only from 0 to 6. After 6 rounds, the target of 10000 rounds is reached, which concludes that the model converges very fast. The training time takes 2 seconds, which indicates that the model has excellent computational efficiency. In terms of performance, the accuracy is from 0.0916 to $7.12e-06$ when the training stops, which is lower than the target value of $1e-05$, and meets the minimum accuracy requirements of the planned model. The gradient from the initial value 0.254 to the stop value 0.00075 is lower than the target value, indicating that the neural network model is close to the optimal solution. The adaptive parameter is reduced from 0.001 to $1e-06$, which indicates that the algorithm is stable and the step size is adjusted reasonably. The validation check value is 0, indicating that there is no overfitting. The R^2 result is 0.99961, indicating that the neural network model fitting results are good. The neural network variance is shown in Fig. 2.

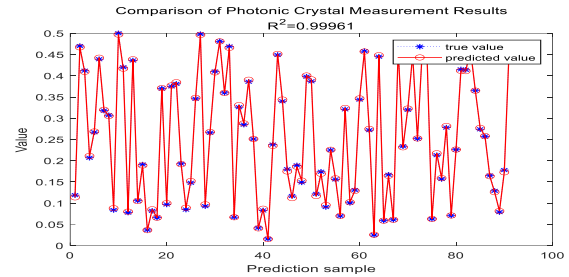


Fig. 2. Neural network variance visualization.

The correlation coefficient of the training set is 0.99983, which is almost a perfect fit. The correlation coefficient of the validation set is 0.99982, which has strong generalization ability. The correlation coefficient of the test set is 0.99986, which shows that this model can also accurately predict unknown data.

The experimental results show that the gradient value of 0.00043958 is far lower than the threshold set by the system $1e-5$, and the model has converged. The damping factor is $1e-6$, which indicates that the model algorithm is close to the Gaussian-Newton method with fast and stable convergence. The verification check value is 0, which means that the verification error does not show a continuous increase and stops early.

In Fig. 3, the variation of training set, test set, and validation set error with the increase of training times is shown.

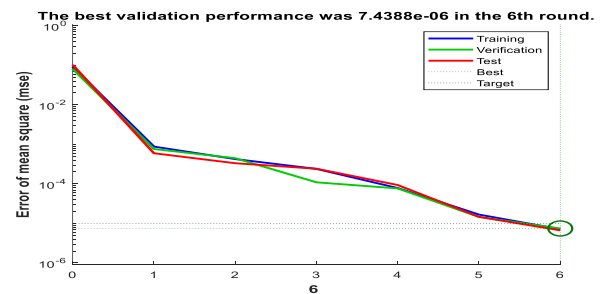


Fig. 3. Sample performance test chart.

VI. CONCLUSION

The goal of this research is to use artificial intelligence neural network to realize the reverse design of photonic crystal structure. The BP neural network is successfully introduced into the design of a photonic crystal microcavity structure, and the inverse prediction model from energy band characteristics to microcavity size is established. Through the study of two-dimensional photonic crystals, it is concluded that BP neural networks can effectively learn the nonlinear mapping relationship between the structure of photonic crystals and their optical properties, and realize the accurate prediction from the target energy band to the structure parameters, with R^2 reaching more than 0.999. Finally, the experimental model can also make accurate predictions for unknown data. In this study, the theory that neural network accurately constructs the quantitative relationship between optical model and optical response is realized, and its artificial intelligence model is applied to the reverse design of optical devices. In this study, due to the experimental equipment, MBP cannot be used to construct more photonic crystal samples for the training of the artificial intelligence network, so that the model can obtain

more accurate predictions. And the design of one-dimensional and three-dimensional photonic crystals has not been constructed. On the basis of this research, training a more predictive ability of artificial intelligence neural network and three-dimensional photonic crystal prediction neural network for the follow-up, this research direction has more important significance. In general, this research direction further frees researchers' time for photonic crystal structure design, and saves money spent on photonic crystal structure experiments.

CONFLICT OF INTEREST

The author declares no conflict of interest.

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