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

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Abstract. To address the high trial-and-error cost and computational workload in defect preparation of two-dimensional photonic crystals, this paper applies a BP neural network to model the relationship between energy band data and defect layer thickness. The dispersion data obtained by the MPB algorithm are used as input, while the defect layer thickness is taken as output. A single-hidden-layer BP neural network is constructed, completing dataset preparation, network design, and model training and testing. Model performance is evaluated using relative error and the coefficient of determination R^2. Results show that the model can rapidly and accurately predict defect layer thickness, with the test set R^2 exceeding 0.92. This significantly reduces computational cost and provides an efficient approach for optimizing photonic crystal microcavity design.

Keywords: MPB algorithm, BP neural network, defect layer thickness, two-dimensional photonic crystal

1. Introduction

Photonic crystals are artificial microstructured waveguide materials with dielectric constants periodically arranged in space. Owing to their unique photonic bandgap properties, they show broad application potential in optical fiber communication, ultra-small laser arrays, and optical integrated devices. As a key type, the size accuracy of defect structures (e.g., microcavities) in two-dimensional photonic crystals directly determines device performance. However, fabrication processes, such as electron beam etching and ultraviolet photolithography, suffer from long cycles and high maintenance costs. Therefore, optimization design prior to fabrication is crucial to reducing trial-and-error costs. Traditional numerical methods, including the plane wave expansion (PWE) method and the finite-difference time-domain (FDTD) method, are widely used in photonic crystal design. Nevertheless, these approaches require parameter sweeps, and the computational burden increases significantly with device size and structural complexity, making rapid design difficult. Artificial neural networks, with strong nonlinear fitting and generalization capabilities, can learn the mapping between inputs and outputs through training data and enable fast prediction of target parameters. As a result, they have been increasingly applied in photonic crystal design. In this paper, two-dimensional photonic crystals are studied. The MPB algorithm is used to compute band dispersion (ω–K) data, and a BP neural network model is constructed to establish the mapping between band characteristics and defect layer thickness. This approach enables rapid prediction of

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defect layer thickness, and its accuracy and stability are verified, providing technical support for efficient defect-structure design.

2. Literature review

Artificial neural networks, with strong capabilities in nonlinear fitting, multi-parameter optimization, and pattern prediction, have become a core auxiliary tool in photonic crystal design, enhancing device performance and structural innovation. Their applications span band analysis, device optimization, and functional expansion.

In studying fundamental characteristics, neural networks provide efficient solutions for bandgap and dispersion analysis. Liu et al. investigated the bandgap structure of two-dimensional photonic crystals using two methods, generating rich training data. By learning mappings among lattice types, dielectric parameters, and bandgap ranges, neural networks can rapidly predict bandgap distributions [1]. Zhong and Yuan addressed energy band structures in two-dimensional dispersive photonic crystals, and their theoretical and numerical results supported neural network training, enabling accurate fitting of optical responses [2]. In functional device design, neural networks enable efficient multi-parameter optimization. Wang et al. developed a two-dimensional photonic crystal wavelength division multiplexer with a double-ring resonator, achieving six-channel multiplexing through iterative tuning; neural networks help shorten optimization cycles based on coupling theory [3]. For 5G applications, 2D cylindrical photonic crystal bandpass filters must meet strict frequency requirements; neural networks can learn relationships among structure, bandwidth, and insertion loss to achieve rapid optimization [4]. Devices such as photonic crystal filters with Kerr media [5] and ring-cavity-based filtering and beam-splitting devices [6] rely on complex parameter control, where neural networks improve design accuracy by learning nonlinear optical characteristics. For functional expansion, neural networks support deeper exploration of photonic crystal properties. Hu's study on localized modes at the Dirac frequency provided data for prediction models [7]. Research on zero-refraction effects [8], device design and analysis [9], and soft X-ray microscopy applications [10] further supplies data for adapting neural networks to diverse wavelengths and functions.

In summary, neural networks play a key role in band analysis, device optimization, and characteristic prediction, and future work should integrate experimental and theoretical data to enhance generalization and practical applications.

3. Design of photonic crystal structure

The two-dimensional photonic crystal studied in this paper uses GaAs as the background material (Figure 1) with a fixed refractive index. Air hole defect structures are periodically arranged, with a refractive index of 1.0 and a base radius of 0.35. The study focuses on the defect layer thickness in the microcavity (radius R), ranging from 0.01 to 0.5 with a step of 0.01, yielding 50 samples. The periodic dielectric structure ensures photonic bandgap formation, while varying defect thickness tunes local properties. MPB is used to compute band structures and obtain ω–K data for neural network input.

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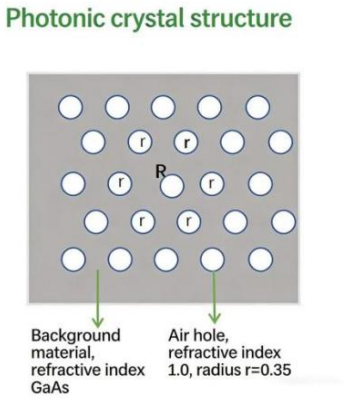

Figure 1. Photonic crystal structure

4. Neural Network Model design

Network Model Selection Considering that a single hidden-layer three-layer BP neural network can approximate any nonlinear function and has a simple structure and high training efficiency, this paper selects a single hidden-layer BP feedforward neural network to establish a mapping model between the two-dimensional photonic crystal band data and the thickness of the defect layer. The model structure consists of an input layer, a hidden layer, and an output layer, as shown in Figure 2.

The BP neural network model consists of three layers. In the input layer, the band dispersion relationship of the two-dimensional photonic crystal calculated by the MPB algorithm is used, where 10 k-points are selected and 8 frequency values from each k-point are extracted, resulting in 80 input features and thus 80 neurons. In the hidden layer, the number of neurons directly affects the model's fitting and generalization ability; after multiple experiments, a single hidden layer with 9 neurons is adopted. In the output layer, the model predicts the defect layer thickness (microcavity radius R), which is a single continuous value, so the number of neurons is set to 1.

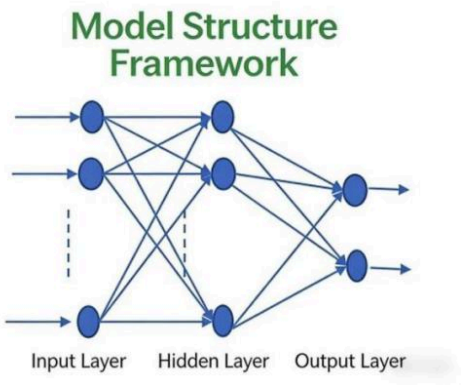

Figure 2. Model structure framework

5. Sample preparation

5.1. Band data calculation

Use the MPB software to write a calculation script, calculate the dispersion relationship of the two-dimensional photonic crystal with 100 sets of different defect layer thicknesses, execute the

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command "mpb p2_loop.ctl|tee p2_loop.ctl.out", extract the TE mode frequency data from the calculation results, and save the band frequency data to a text file using "grep tefreqs p2_loop.ctl.out> p2_loop.dat", providing a basis for subsequent data preprocessing.

5.2. Data preprocessing

Due to the presence of null values (NaN) in the original calculation data, data cleaning is first performed, followed by feature extraction and sample construction. Specifically, MATLAB is used to read the data file, and all empty rows are detected using "all(isnan(data), 2)" and removed to obtain a clean band data matrix. Then, frequency feature data from columns 6 onward are extracted and grouped by defect layer thickness, with each group containing 10 k-points and 80 frequency values. Next, the 80 frequency values of each group are reconstructed into a one-dimensional row vector as the input sample, with the corresponding defect layer thickness as the output. Finally, 100 valid samples are generated and saved as "p1_dataset.mat."

5.3. Training set and test set division

To ensure the generalization ability of the model, the samples are randomly divided into a training set and a test set, following the principle that the training set accounts for 80% and the test set accounts for 20%. Randomly select 80 sets from the 100 samples as the training set for model parameter training; the remaining 20 sets are used as the test set to verify the prediction performance of the model, ensuring that the sample distribution patterns of the training set and the test set are approximately consistent.

6. Network model training and testing

6.1. Data format conversion

Load the sample data file "p2 dataset.mat" in the MATLAB environment. Transpose the input feature matrix "inputdata" and the output label vector "r" to make each column correspond to a sample and each row correspond to a feature, which meets the input data format requirements of the BP neural network. Define the transposed input data as "Input" and the output data as "Output".

6.2. Model training and simulation testing

In model training and simulation testing, random indices from 1 to 100 are first generated to shuffle the samples and avoid sequence effects on training results. Then, the first 80 groups are used as the training set ("P train" and "T train"), while the remaining 20 groups form the test set ("P test" and "T test"). A single-hidden-layer BP neural network is constructed using "feedforwardnet(9)" with preset parameters, and trained via "net = train(net, P train, T train)," during which error curves and gradient changes are monitored until convergence. Finally, "P test" is input into the trained model to obtain "T sim bp," which is compared with "T test" for performance evaluation.

6.3. Performance evaluation indicators

Use relative error and coefficient of determination R^2 as the quantitative evaluation metrics for the model performance. Among them, the relative error reflects the prediction accuracy of a single

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sample, while, R^2 reflects the overall fitting degree of the model. The closer it is to 1, the better the prediction effect of the model.

As shown in Figure 3, after the model training of the test results was completed, the prediction results of the test set showed that the relative error of the model was controlled within a reasonable range, and the coefficient of determination R^2 of 0.92305. This indicates that the built BP neural network model can effectively fit the nonlinear relationship between the two-dimensional photonic crystal band data and the thickness of the defect layer, and achieve precise prediction of the defect layer thickness. By drawing the comparison curve of the true values and predicted values of the test set, it is possible to visually observe that the trend of the predicted values and the true values is highly consistent, further verifying the effectiveness of the model.

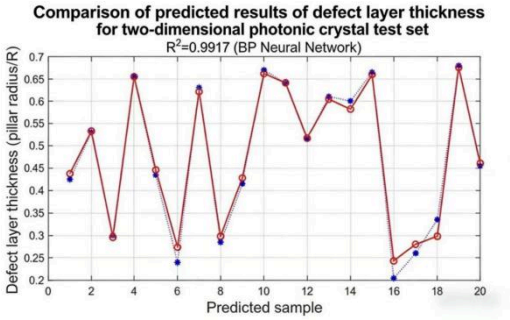

Figure 3. Comparison of predicted results of defect layer thickness for two-dimensional photonic crystal test set

6.3.1. Performance

Figure 4 illustrates the changes in mean squared error (MSE) of the training, validation, and test sets during the 8 rounds of model training. The error decreased rapidly in the initial stage and reached the minimum value of 0.0002187 on the 2nd round of the validation set. Subsequently, it converged to the order of 10^{-4}, indicating stable performance without significant overfitting or underfitting.

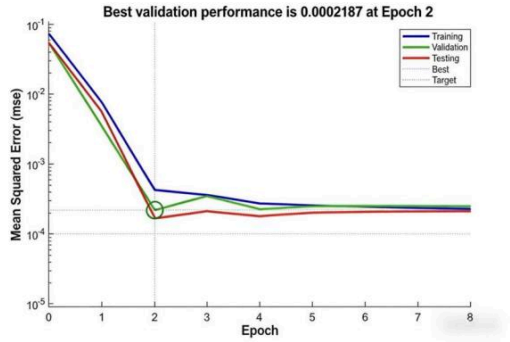

Figure 4. Best validation performance is 0.0002187 at Epoch 2

6.3.2. Training status

The gradient rapidly converges to 0.0039794; the Mu parameter fluctuates periodically initially and then remains constant at 0.001; the number of validation checks gradually increases to 6, indicating that the model is approaching the convergence limit.

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6.3.3. Regression

Figure 5 shows the target-output fitting graph for training, validation, testing, and the entire dataset. The correlation coefficients R for each subset are 0.98838, 0.99538, 0.997, and 0.99101, respectively. The fitted line closely coincides with the ideal line Y = T, indicating excellent prediction accuracy and stable generalization ability of the model.

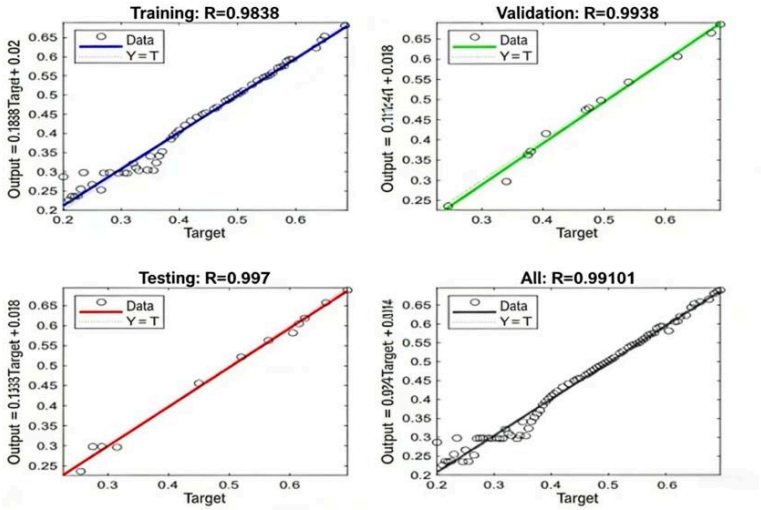

Figure 5. Target-output fitting plots

7. Conclusion

This paper applies the BP neural network algorithm to predict the defect layer thickness in two-dimensional photonic crystals. Based on band dispersion data calculated by the MPB algorithm, sample preparation, network design, and model training and testing are completed. The results show that MPB efficiently provides band characteristic data, which, after cleaning and reconstruction, are transformed into high-dimensional input vectors suitable for neural network modeling, ensuring reliable training data. The single-hidden-layer BP neural network (high-dimensional input, 9 hidden neurons, 1 output neuron) successfully establishes the nonlinear mapping between band data and defect layer thickness, with stable convergence. The test set determination coefficient R^2 exceeds 0.92, indicating high prediction accuracy. Compared with traditional methods such as PWE and FDTD, the trained BP neural network enables rapid prediction without repeated parameter sweeps, significantly reducing computational cost and time. This study offers an efficient method for defect structure design. Future work can further improve accuracy and generalization by expanding sample size, optimizing network structure, and integrating multi-dimensional features.

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