

BP neural network model for reverse design of two-dimensional triangular lattice photonic crystals

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Abstract:

By learning the related properties of photonic crystals, two-dimensional photonic crystals with triangular lattice are selected for study. The point defects are set up and the photon band calculation is carried out by using MPB. The calculated sample data is imported into MATLAB, and the relationship between point defects and photonic energy bands is found by building Bp neural network model, which provides a new method to solve the reverse design of photonic crystals.

Key words: Photonic crystal, two-dimensional, triangular lattice, Bp neural network

1. Instruction

The concept of photonic crystals was first proposed by Yablonovitch of Bell Laboratories in the United States and John of Princeton University in 1987 and extensively studied^[1-2]. A photonic crystal is an artificial periodic dielectric structure known for its photonic band gap arranged in one, two or three dimensions. In photonic crystals, the periodicity of different dielectrics in space has a regulatory effect on the propagation of light, which is due to the change of spatial arrangement resulting in Bragg Scattering, which makes the photon band gap appear when the light wave propagates in it, and the light falling into the band gap will not be able to continue to propagate, also known as "photonic band gap".

The main factor influencing the generation and size of photonic crystal band gap is its effective refractive index n_{eff} , which is generally achieved by changing the shape and size of photonic crystal dielectric column, dielectric constant of dielectric column and background, etc. The theoretical design and search for photonic crystal structures with wider bandwidths has always been one of the important research directions in this field

Photonic crystals have unique advantages in physical properties and great prospects for application and development. The preparation and application of photonic crystals have long been the focus of academic research. In the context of microwave technology, photonic crystals have been applied in the production of microwave resonator, microstrip antenna, mixer and other microwave devices^[6]. Because the preparation of three-dimensional photonic crystals is very difficult, people pay more attention to the

preparation of two-dimensional photonic crystals.

Therefore, our research object will also focus on two-dimensional photonic crystals, and use Bp neural network model to address the problem of reverse design of photonic crystals.

2. Model selection

In the current study of two-dimensional periodic media structures, two-dimensional photonic crystals composed of triangular lattices have become the focus of research.

The triangular lattice finds extensive applications in the employed and manufacturing of two-dimensional photonic crystals due to its inherent structural advantages^[7-8]. Currently, the triangular lattice structure has been successfully employed in various photonic devices such as light-emitting diodes, lasers, and fibers^[9-11]. Previous studies have demonstrated that arranging air cylinders using a triangular lattice structure can lead to the achievement of a significant complete photonic band gap^[9]. Furthermore, incorporating regular hexagon air cylinders within the dielectric background has been discovered to generate another complete photonic band gap^[12-13]. Additionally, researchers have also observed the presence of a photonic band gap in the triangular lattice structure composed of square GaAs dielectric columns with varying widths^[14], and the maximum bandgap width is

$$\Delta_{\max} = 0.0136 \times \frac{\omega\alpha}{2\pi}$$

Where ω is the angular frequency of electromagnetic wave, α is the photonic crystal lattice constant and c is the speed of light.

Therefore, this time we will also use two-dimensional photonic crystals with triangular lattice structure for research, and the structure diagram is as follows:

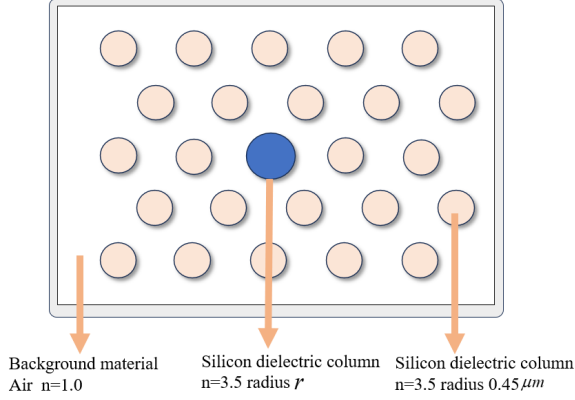


Fig 1: Schematic diagram of two-dimensional photonic crystal structure with point defects

The chosen background material for this study was air, which possesses a refractive index of approximately 1. A silicon-based dielectric column with a radius of $0.45 \mu\text{m}$ and a refractive index of around 3.5 was employed. Throughout the experiment, the intermediate dielectric column consistently maintained its refractive index at the value of 3.5.

3. Back Propagation Algorithm

3.1 BP Algorithm

The BP algorithm is a learning method that uses mean square error and gradient descent to modify network connection weights. The purpose of modifying these weights is to minimize the sum of squared errors. In this algorithm, a smaller value is initially assigned to the network's connection weights. Then, select a training sample and calculate the gradient of the error relative to that sample^[15]. This time, we will use the above BP neural network model to establish a model of the relationship between point defect radius and photonic crystal dispersion to solve the problem of photonic crystal reverse design.

3.2 Description of BP Algorithm in Mathematics

To modify the weights and thresholds in the direction opposite to the negative gradient is what behind the learning rules of the BP network. We need to find the direction which indicates the fastest rate of decrease.

In a three-layer BP neural network, we have input nodes denoted as m_j , hidden layer nodes denoted as n_j , and output layer nodes denoted as l_j . We use ω_{ji} to represent the weights on the input nodes connected to the hidden layer nodes, and the weights connecting the hidden layer

nodes to the output layer nodes are represented as η_{ij} . The desired output value for the output node is o_l , and the activation function is $g(\cdot)$.

The computational formula of this model are expressed as follows:

Output of the node of hide layer

$$y_j = g\left(\sum_i \omega_{ji} m_i - \varepsilon_j\right) = f(o_j)$$

$$\text{including } o_j = \sum_i \omega_{ji} m_i - \varepsilon_j$$

The computational result of the output node

$$l_j = g\left(\sum_j \eta_{ij} n_j - \varepsilon_l\right) = f(o_l)$$

$$o_j = \sum_i \omega_{ji} m_i - \varepsilon_j$$

Including

error of the output node

$$\begin{aligned} E_r &= \frac{1}{2} \sum_l (o_l - l_l)^2 = \frac{1}{2} \sum_l (o_l - g(\sum_j \eta_{lj} n_j - \varepsilon_l))^2 \\ &= \frac{1}{2} \sum_l (o_l - g(\sum_j \eta_{lj} g(\sum_i \omega_{ji} m_i - \varepsilon_j) - \varepsilon_l))^2 \end{aligned}$$

Back propagation involves employing the gradient descent method to adjust the weight values in all layers.

This time, we will use the BP neural network model to establish a model of the relationship between point defect radius and photonic crystal dispersion to solve the problem of photonic crystal reverse design.

4. MIT Photonic-Bands

The energy bands of photonic crystals in this study were calculated using the software MIT Photonic-Bands (referred to as MPB), developed by Steven G. Johnson, a researcher from the Ab Initio Physics Group at Massachusetts Institute of Technology specializing in photonic crystal research. The program operates on Linux platforms and is distributed under the GNU General Public License, enabling global collaboration, knowledge exchange, and academic advancement among researchers in the field of photonic crystal research.”

The MPB software package is specifically designed to compute the finite-frequency characteristic states of the Maxwell equations in periodic media, making it a valuable tool for determining band gaps of optical wave modes in structures with periodic media. However, its applications extend beyond this scope and encompass calculating dispersion relations and characteristic states in optics, such as photonic crystal fibers.

In this study, we will use MPB software to write code to

calculate the dispersion relationship of two-dimensional photonic crystal with point defects, and get sample data under different radii through circulation.

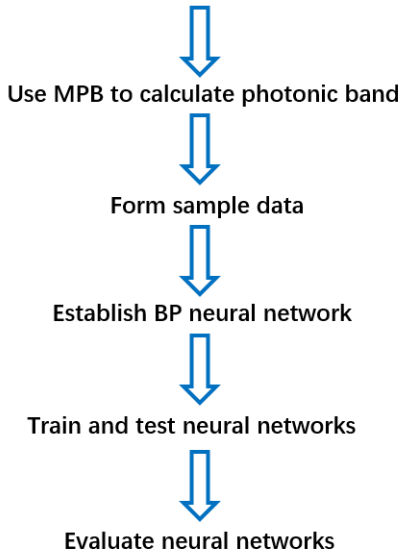
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Creating Meshell data...
Mesh size is 3.
Lattice vectors:
(1, 0, 0)
(0, 1, 0)
(0, 0, 1)
Cell volume = 1
Reciprocal lattice vectors ( / 2 pi ):
(1, 0, 0)
(0, 1, 0)
(0, 0, 1)
Geometric objects:
cylinder center: (0,0,0)
radius: 0.2, height: 0.2, axis: (0, 0, 1)
position: 1, n = 1
Geometric object tree has depth 1 and 1 object nodes (vs. 1 actual objects)
Initializing option function...
Allocating fields...
# k points:
(0, 0, 0)
(0, 2, 0, 0)
(0, 2, 0, 0)
(0, 2, 0, 0)
(0, 2, 0, 0)
(0, 2, 0, 0)
(0, 2, 0, 0)
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Solving for band polarization: te
Initializing fields to random numbers...
Elapsed time for initialization: 0 seconds
maxfun: 1, 12, 7, mean: 20229, error: mean 1.0448, 14.5580n = 1, 12, 5663n 'fill'
Submitting for MPI-parallel...
solve bands: (0, 0, 0)
kfreqs: k index, k1, k2, k3, kfreq/zpl, te band 1, te band 2, te band 3, te band 4, te band 5, te band 6, te band 7, te band 8
Solving for bands 2 to 8...
l1min: converged after 7 iterations.
l1min: converged after 8 iterations.
l1min: converged after 8 iterations.
l1min: converged after 8 iterations.
l1min: converged after 4 iterations.
l1min: converged after 3 iterations.
l1min: converged after 4 iterations.
l1min: converged after 4 iterations.
l1min: converged after 4 iterations.
l1min: converged after 4 iterations.
l1min: converged after 4 iterations.
l1min: converged after 4 iterations.
    
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Fig 2: Schematic diagram of the MPB software calculating the photon band

5. Research process and results

radius of photonic crystal microcavity $r=0.00:0.01:0.5$



We first set the point defects for the selected triangular lattice photonic crystal by changing the size of the microcavity of the photonic crystal, and then use MPB to write a code to calculate the photonic band. The calculated sample data is imported into MATLAB and the Bp neural network model is established by using the written Bp neural network code.

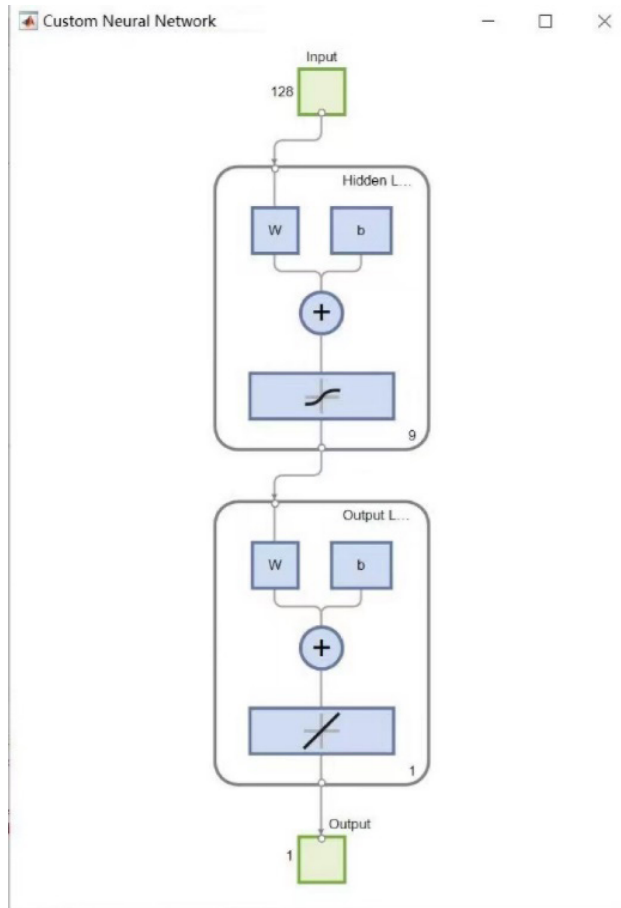


Fig 3: Schematic of the neural network setup Through the continuous testing and training of the neural network, we get the following results and evaluate the established Bp neural network model.

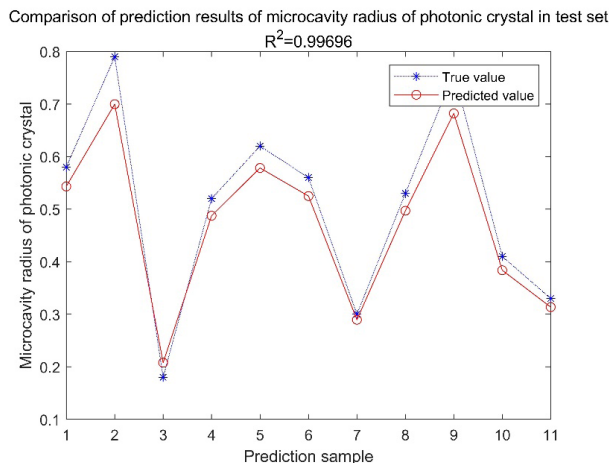


Fig 4: Comparison of prediction results of microcavity radius of photonic crystal in test set

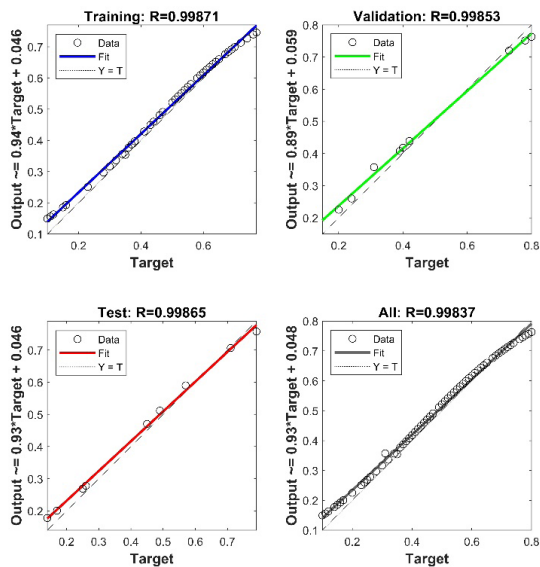


Fig 5: R-square result graph

As can be seen from the above two figures, the effect of neural network establishment is relatively ideal, and the R square is 0.99 very close to 1, indicating that the regression effect is very good. We can use this model to know how to set the radius of the point defect to achieve the desired photon band.

6. Prospect

Through our research, we can find that it is feasible and meaningful to use BP neural network model to address the problem of reverse design of two-dimensional photonic crystals. At present, we only set point defects for two-dimensional photonic crystals of one structure. In the future, more Settings for defects can be carried out, and this model can be applied to two-dimensional photonic crystals with different structures to solve more reverse design problems of photonic crystals, and improve the flexibility and diversity of reverse design.

7. Reference

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