Prediction of Topological Invariants in Photonic Crystals Using Machine Learning

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Abstract— Artificial neural network is a mathematical model or computational model that mimics the structure and function of biological neural networks and is used to estimate or approximate functions. We train the artificial neuron network with the dataset based on the structural and material parameter with special method to predict the geometric phases of some certain bands in 1D photonic crystals. It shows that the well-trained network can accurately predict the topological characteristics of the band structure and has good adaptability and adjust-ability for more complex structural parameters of the photonic crystal. At the same time, the use of the network can improve the efficiency of the calculation for photonic crystal topological properties and lay a good foundation for the reverse design of photonic crystal materials.

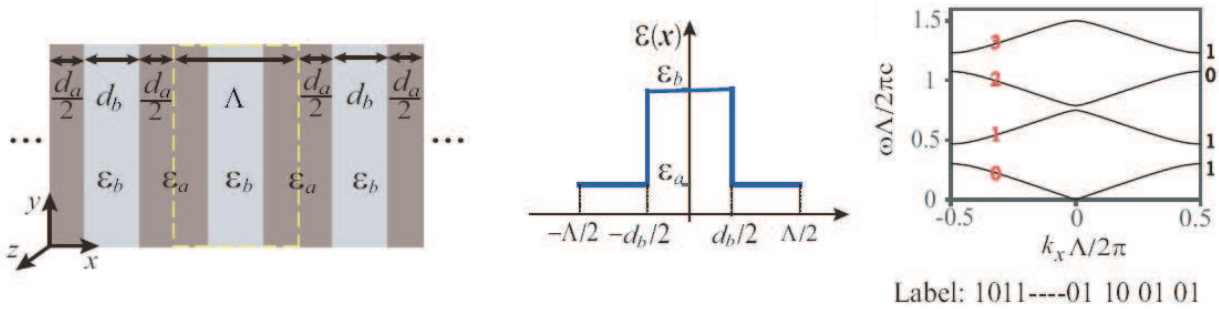
1. INTRODUCTION

Recently, machine learning and deep learning techniques based on artificial neural network analysis has been applied to many fields and has attracted a lot of interest on the corresponding practical problem, such as image recognition [1] and speech transcription [2], which makes many problems that are difficult to be solved by traditional algorithms have obtained efficient and accurate results. The achievement of neural networks (NNs) mainly depends on its ability to make a good connection between input and output, that is to say, 'inference'. The benefit of NNs also makes it used to solve the hard problems in the field of optics and photonics. In optics, there have been a lot of works about utilizing the NNs for the design of multi-layered thin films [3], meta-surfaces [4], and multilayer nanoparticles [5]. Moreover, some recent works have attempted to design the topological photonics [6, 7] and predict the physical quantities on condense matter physics [8]. Topology has recently been recognized as an important concept in physics, as evidenced by the recent development in topological materials, as well as different forms of topological protected phenomena. In order to obtain the topological phase of the topological structures often requires a lot of complicated calculation. The NNs can be used to predict topological phase to simplify the process.

In this work, we firstly train the NN with the dataset directly using the structural and material parameters to predict the topological phases of the bands for the 1D PC. Secondly, we train the NN with the dataset with the input of dielectric distribution on one unit in 1D PC. By comparing the results for these two NN, it can been found that the dielectric distribution is more conducive to neural networks to learn the topological properties of the corresponding PC.

2. THE STRUCTURE OF PHOTONIC CRYSTAL AND NEURAL NETWORK

Specifically, considering an AB layered PC illustrated in Fig. 1(a) with the unit cell marked by yellow dashed box. The dielectric constant of A(B) layer is $\varepsilon_a(\varepsilon_b)$, the relative permeability of A(B) layer is $\mu_a(\mu_b) = 1$ and the thickness of A(B) layer is $d_a(d_b)$. The lattice constant $= d_a + d_b$ is fixed throughout this work. As shown in Fig. 1(b), the dispersion of the lowest four bands (solid lines) calculated using the transfer matrix method (TMM) [9, 10], with parameters $\varepsilon_a = 4$, $\varepsilon_b = 1$, $d_a = 0.3\Lambda$, $d_a = 0.7\Lambda$. As the system has inversion symmetry, the geometric Zak phase of each Bloch band is either 0 or 1, with a corresponding winding number of 0 or 1. We calculate the Zak phases of the bands and label each band with its winding number, in Fig. 1(b). As for the label of the bands considered in this paper, for example, the four-binary-number labeling is translated into a decimal integer, e.g., 1011 in Fig. 1(b) to 01100101 for convenience for the output of the NN,



(a) (b) (c)

Figure 1: (a) The structure of an AB layered photonic crystal. The yellow dashed box shows the unit cell with lattice period Λ. (b) The band dispersion of the structure with parameters $\varepsilon_a = 4$, $\varepsilon_b = 1$, $d_a = 0.3\Lambda$, $d_a = 0.7\Lambda$. (c) The distribution of the dielectric constant in one unit.

with 01/10 corresponding to the winding number 1/0. In Fig. 1(c), the distribution of the relative permittivity $\varepsilon(x)$ in one unit cell $[-\Lambda/2, \Lambda/2]$.

In order to train the NN, we need to build datasets. For convenience, we firstly keep the midgap position unchanged, i.e., $n_a d_a + n_b d_b$ should be a constant, set as C, where $n_a = \sqrt{\varepsilon_a \mu_a}$ and $n_b = \sqrt{\varepsilon_b \mu_b}$. Once this constant is fixed, with the constrains $d_a + d_b = 1$ and $\varepsilon = 1$. Supposing the $C = 1.4$, the variable $\varepsilon_a \in (3, 10)$ is the rang for the samples in training dataset and the variable $\varepsilon_a \in (2, 15)$ is the range for the samples in training dataset. The samples in those ranges is random. For one sample, we can get four parameters $(\varepsilon_a, \varepsilon_b, d_a, d_b)$ and characterize the topological phases for the bands in the way shown in Fig. 1(b).

Then we introduce the workflow of our NN, as shown in Fig. 2. The NN has four layers with yellow, green and blue neurons, corresponding to the input, hidden and output layers, respectively. We have three ways to prepare the input data for the input layer. 1) Feeding the NN directly with the structural and material parameters, the input layer has four neurons representing $(\varepsilon_a, \varepsilon_b, d_a, d_b)$. 2) We divide the unit cell into 100 pieces and obtain a discrete array value ε_i, $i = 1, 2, ..., 100$, with $\varepsilon_i = \varepsilon_a$ or ε_b. for this case, the input layer should be 100 neurons. 3) In order to further improve the accuracy of division, the i in 2) can be increased to 500, corresponding to the 500 neurons of the input layer. In other words, we select three different input networks, namely with 4 neurons, 100 neurons and 500 neurons of input layer. The output layer is represented the topological properties the NN should learn, whose labels we have mentioned above, and the number of its neurons depends on the topological bands we choose. The hidden layers will be modified to obtain the better performance. The number of hidden layers and neurons indicated in Fig. 2 does not necessarily represent the number of layers required for actual training and the number of neurons.

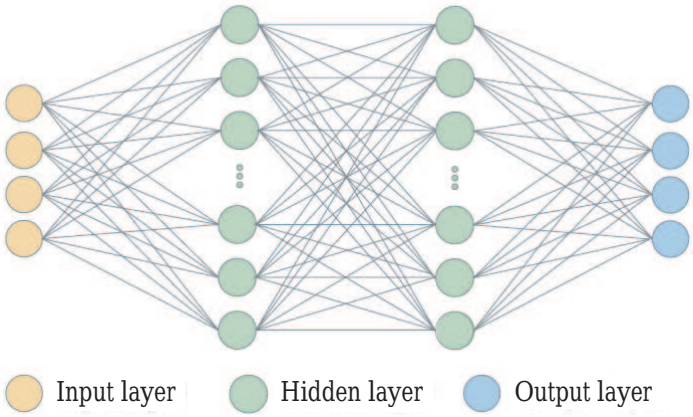


Figure 2: Sketch of the neural network with four layers, consisting of one input layer, one output layer and two hidden layer. The input layer represents the information of the structural and material parameters.

3. PERFORMANCE OF THE NEURAL NETWORK TO LEARNING THE TOPOLOGICAL PHASES

We firstly train the NN of the input layer with 4 neurons with the training dataset, and utilize the labels of the 0 band (the lowest band) and the 1st band (the second lowest band) as a reference to the output of the network to evaluate the performance network. At the same time. The same procedure is applied to the other two network settings, and the cross entropy the predicted topological phase information of the network output and between the labels are used as the loss function. The detail accuracy results for all the NNs are depicted in Table 1.

Table 1: The accuracy results of the NNs based on different inputs and different bands with $C = 1.4$.

	band 0 and 1			band 2 and 3		
number of input neurons	4	100	500	4	100	500
Training accuracy	97.12%	100%	100%	88.5%	99.12%	99.12%
Test accuracy	97%	100%	100%	86%	92%	92%

Form the comparison between the there networks based on the topological phases of the 0 band and the 1st band, the input data with the form of distribution array is better for the NN to learning the topological information, due to the accuracy results for the NN with 4 neurons is 97.12% for training and 97% for test, both below to these for 100 and 500 neurons. For the training based on the 2nd band and the 3rd band, due to the situations of the topological phases on those two band are more complicated than the lowest two band, so the whole accuracy is below to the accuracy for the training based on the lowest two bands. As for the way of the input, it is once again proved that the distribution of materials used to train is more beneficial to train with directly giving parameters with the 88.5% accuracy for 4 neurons and 99.12% for 100 neurons. As for the reason that the accuracy of training with 100 or 500 neurons is 7% larger than that for test, it can be attributed to that there are new topological phases occurred in test dataset.

4. CONCLUSION

To conclusion, we design, train and test the NNs with derectly feeding the structural and material parameters or the distribution function, and it is can be seen that the NNs have a good performance to predict the topological phases of the bands for the 1D PCs. As for the comparison on the input formats, the input for the NNs should be more concrete, and it will helps the NN to obtained the more accurate results.

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