Inverse Design of Photonic Crystal Nanobeam Cavity Structure via Deep Neural Network

Jianjun Hao, Lei Zheng, Daquan Yang, Yijun Guo*

Beijing Key Laboratory of Network System Architecture and Convergence, Beijing University of Posts and Telecommunications, Beijing, 100876, P. R. China. jjhao@bupt.edu.cn, zhenglei@bupt.edu.cn, ydq@bupt.edu.cn, *guoyijun@bupt.edu.cn

Abstract: We propose a deep learning framework to solve the inverse design problem of one-dimensional photonic crystal nanobeam cavity structure. After training, we obtained an effective solution to the inverse design. © 2019 The Author(s)

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1. Introduction

In nanophotonic, inverse design from given optical responses to geometric structure is a challenging problem, since it needs complicated calculation [1]. The traditional way to solve the inverse problem can be summarized into two categories [2]. The first is genetic algorithm. The electromagnetic response is used to iterate parameters which is initialized randomly and match desired spectrum continually. On running genetic algorithm, we spent more computing resources and time to ensure the structural requirements. The second is the adjoint method. We established an inverse mathematical model by solving adjoint equations to get desired parameters. Adjoint equations may have no analytical solution though the adjoint method seems to be more efficient than the genetic algorithm. However, the iteration and optimization process of these methods are time-consuming and prohibitively slow, due to the high non-linearity of the inverse design.

As structure size and complexity grow, traditional numerical optimization methods becomes complicated and impossible. Data-driven methods based on deep learning which can uncover unknown relations among a huge number of variables emerges [2–4]. With a well-trained deep neural network (DNN), a possible structure corresponding to a given spectrum can be computed rapidly, which outperforms complicated traditional numerical optimization methods. For example, Peurifoy et al. combined deep learning with nanophotonics to predict the shell-shaped nanophotonics [2]. Liu et al. applied neural network to predict thin-film nanostructures successfully [3]. Ma et al. used CNNs to predict the structure of chiral metamaterials [4].

In recent, ultra-high Q-factor (Q) and ultra-low mode volume (V_m) one-dimensional photonic crystal nanobeam cavities (1-D PCNC) have emerged as an advantageous platform for on-chip nanophotonics, including quantum optics, integrated nanophotonics and optical tweezer [5, 6]. In this paper, a DNN is proposed to solve the inverse design problem of 1-D PCNC and verify its accuracy by comparing with electromagnetic simulations. We focus on 1-D PCNC whose thickness is ignored, as shown in Fig.1. Ten circular micro-cavities are arranged laterally and



Fig. 1. The structure of 1-D PCNC.

symmetrically in a two-dimensional space. Denote the center distance between adjacent cavities as period a, the radius of central cavity as R_c and the radius of edge cavity as R_e . Then an 1-D PCNC structure could be completely determined by a, R_c and R_e . The laser goes into the cavity horizontally from one side. The transmission spectrum which is called the fundamental mode(FM) is different according to different structural parameters. The shape of FM is shown in Fig.2(a).

2. Results and Discussion

A DNN as shown in Fig.2(b) is trained to study the hidden relationship between the structures and spectrums of 1-D PCNC. With desired spectrum entered into input layer and passed through three hidden layers, the intermediate layer outputs the predicted structure parameters, which is entered into another three hidden layers, and the last layer outputs the predicted spectrum finally. The loss function *L* consists of two parts, being written as eq.(1):

$$L = L_{struct} + L_{spect} \tag{1}$$

 L_{struct} denotes the MSE between desired structure and predicted structure. L_{spect} denotes the MSE between the desired spectrum and the predicted spectrum. Our end-to-end network is different from others without stacking training, which improves training efficiency significantly.



Fig. 2. (a) The FM of 1-D PCNC. (b) Construction of deep learning model.

For a given desired spectrum, we compare the structure predicted by DNN and computed by simulation. As shown in Fig.3(a), the three structure parameters obtained from two methods are nearly the same. Further, we compare the corresponding spectrums as shown in Fig.3(b). The resonance peak calculated from system spectrum



Fig. 3. (a) The retrieval parameters of 1-D PCNC. (b) The transmission spectrum of 1-D PCNC(FM).

by the predicted structure is consistent with that calculated from simulation spectrum. The error of resonance peak between DNN method and simulation is less than 3nm. The error of resonance peak between DNN method and desired spectrum is less than 5nm. The results verify that the proposed DNN method is able to complete inverse design with an acceptable margin of error. However, compared to time-consuming methods, DNN method can accomplish the design goal in a fraction of second.

In this work, we propose a DNN and demonstrate its powerful ability of predicting 1-D PCNC parameters. By the means of this special network, we solve the inverse design problem of 1-D PCNC that is difficult for traditional methods. Our innovative research makes sense of the application for other nanophotonic structures. By the same token, our further researches will concentrate on improving our network architecture for the inverse design of nanophotonic structures to get better accuracy.

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