A novel guided deep learning algorithm to design low-cost SPP films

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Abstract

The design of surface plasmon polaritons (SPP) films is an ill-posed inverse problem. There are many-to-one correspondence between the structures and user needs. We present a novel guided deep learning algorithm to find optimal solutions (with both high accuracy and low cost). To achieve this goal, we use low cost sample replacement algorithm in training process. The deep CNN would gradually learn better model from samples with lower cost. We have successfully applied this algorithm to the design of low-cost SPP films. Our model learned to replace precious metals with ordinary metals to reduce cost. So the the cost of predicted structure is much lower than standard deep CNN. And the average relative error of spectrum is less than 5%. The source codes are available at https://github.com/closest-git/MetaLab.

Keywords: deep learning, inverse design, sample replacement algorithm, low-cost photonics device

1. Introduction

Surface plasmon polaritons (SPP) are two-dimensional electromagnetic waves confined at the metal–dielectric interfaces [1]. They can be used to break the diffraction limit, which is very important for many areas such as information storage, biosensing, and integrated photonic circuits [2]. But the inverse design of SPP structures is an ill-posed inverse problem[3]. There are many-to-one correspondence between the structures and user needs. Users not only want to get a solution, but also need the solution to be optimal on some criterion or some cost function. This is the key problem of inverse design process.

We mainly investigate low-cost multilayer metal/dielectric nanocomposite films that support surface plasmon polaritons. Usually users want SPP at specified incident angle and wavelength, which could be described by two dimensional reflectance map. The most used metal types are gold (Au), silver (Ag), copper (Cu) and aluminium (Al). The cost of Au is much expensive than Ag, Cu and Al. So not only the films’ spectrum should meet the users’ requirements, but the lower the cost, the better. That is, user want to design films with as less as possible. Recently, machine learning methods show great power in design nano-photonics[4-9]. But all these models do not take cost factor into account. The predicted design result may have much higher cost than the optimal solution. No other teams find ways to tackle the cost problem by deep learning. In this paper, we present novel guiding mechanism for this problem, which will guide CNN from training samples with lower and lower cost. And it not only predicts a solution with high accuracy, but also find much lower cost solution. To our knowledge, It’s a first step in the low cost inverse design problem by deep learning.

Compared to recent works [13-24] of other teams, we use two dimensional response maps instead of one dimensional spectra curves, which are used by nearly all other teams. To our knowledge, it’s the first attempt to use 2D map as training samples. 2D map have much more details. More importantly, we can use deep convolutional neural networks (CNN). Although all teams adopt the framework of deep learning, most other teams use classical deep multi-layer perceptions (MLP). While we use deep CNN to train these 2D maps. Deep CNN has much stronger recognition and discrimination ability than classical MLP. Since CNNs have convolution and pooling layers to exploit spatial invariance. If we use MLP to train image, the images have to be flattened and lost spatial information. Also, CNNs share weights in the convolutional process to cut down on the number of parameters, which makes them extremely efficient in image processing, compared to MLPs.

We also have made breakthroughs in the following two novel points. 1) We use novel guided algorithm in training processes, which would work for any user-need cost functions. This method would meet users’ guideline. The author of [14] raised an important question: “The lack of design guidelines for data-driven methods to deal with.” Our novel guided algorithm is the first attempt to answer this question and get good results. 2) We use hybrid network to solve both classification and regression problem. Similar scenes are often encountered in the inverse design of nanophotonics structures. For example, [15] employed
another network to classify the spectra of different nanostructures. Single hybrid network would reduce the training time and the size of model greatly compare to two independent networks. Our approach showed the potential of hybrid network, which could apply to other similar problems.

2. Methodology

2.1. 2D spectrum

We use deep CNN to learn 2D spectrum of SPP films. This is the one of main difference between us and [4-9]. All backbones of neural networks in [4-9] are classical multilayer perceptrons (MLP) and the inputs are 1D spectrums. Deep CNN uses much more complex structures and have much more powerful ability to learn features than simple MLP. Figure 1 showes some 2D reflectance spectrums of SPP multilayer films, which generated by the characteristic matrix method [10]. We can see the dips, lengths and ranges of SPP curves in the 2D reflection spectrum and other detail information, which could be analyzed by deep CNN. The generation process of 2D spectrum is as following:

\[
\mathbf{M} = \begin{bmatrix}
\cos \delta & \left( j / \eta \right) \sin \delta \\
\eta \sin \delta & \cos \delta
\end{bmatrix}
\]

All intermediate matrices are then multiplied to get the total matrix:

\[
\mathbf{M}_\text{total} = \mathbf{M}_2 \mathbf{M}_3 \cdots \mathbf{M}_{k-1}
\]

Let \( \mathbf{M}_\text{total} = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} \), then the reflection coefficient of the entire multiple-layer structure is

\[
\rho = \frac{\eta_1 (m_{11} + m_{12} \eta_k) - (m_{21} + m_{22} \eta_k)}{\eta_1 (m_{11} + m_{12} \eta_k) + (m_{21} + m_{22} \eta_k)}
\]

For each incident angle \( \delta \) in the range \([0^\circ \sim 90^\circ]\), we get 1D reflectance curve \( \rho \) at different wavelengths from 300nm to 2000nm. Then we merge these curves along Y axis to generate 2D spectrums.

2.2. Guided Training of Cascaded CNN

In view of machine learning, we define the training data \( D=\{ (O_i, Y_i), i = 1, 2, \cdots, M \} \), where each \( O_i \) represents a specific 2D spectrum, \( Y_i \) represents structure parameters of multilayer films (thickness and material type of each layer). The learning algorithm is described by a function \( f(\rho, Y; \Theta) \) parameterized by \( \Theta \), which is expected to fit the training data well and have good generalization for the testing data. In the framework of deep learning, \( \Theta \) includes deep convolutional neural network(CNN) and other task specified modular. In this paper, we present a novel Guide-Resnet architecture as shown in figures 2. The backbone of Guide-Resnet is classical residual network Resnet-18[11]. Resnet-18 has powerful representational ability to extract features from 2D spectrum. But in classical training process of deep CNN, there is no way to lower down the cost of
samples. So the learned model does not take price into account. The predicted design result may have much higher cost than the optimal solution. We enhance Resnet-18 with guiding mechanism to find low cost solutions.

Network architecture

The Guide-Resnet is composed of stacked entities with identity loops referred to as modules. Each module consists of a multiple convolutional layers to learn the features in the input spectrum. A typical module gets input x and generates F(x) through pairs of convolutional and ReLU layers. The generated \( F(x) \) is then added to the input \( x \) which is computed as \( F(x) = F(x) + x \). We keep the max pooling to \( 3 \times 3 \) with the stride of \( 2 \times 2 \). We use Softmax after fully connected layers as default. We use Adam optimizer is a memory efficient and faster computing optimization technique, which is based on adaptive estimates of lower-order moments.

Low cost sample replacement algorithm

We use low cost sample replacement algorithm in training process to find optimal solutions. For each sample in training set \((O_i, Y_i)\), let \( Y_i \) is its original structure (thickness and material type of each layer); \( O_i^0 \) is its original 2D map; \( c_i^0 \) is its cost. In each step of training process, the network would get new output \( \tilde{Y}_i \) (thickness and material type of each layer). Generally, the corresponding structure of \( Y_i \) and \( \tilde{Y}_i \) is different. We pick low cost sample as following:

Generate new 2D map \( \tilde{O}_i \) and its cost \( \tilde{c}_i \) on the structure of \( \tilde{Y}_i \). If \( \tilde{O}_i \) nearly the same as \( O_i^0 \), and \( \tilde{c}_i \) is lower than current \( c_i \), then \( \tilde{Y}_i \) is valid low cost sample.

For each low cost sample, we replace its original sample \((O_i, Y_i)\) by \((O_i, \tilde{Y}_i)\). So in the later training process, the average cost of training set will gradually decline, while spectrum remains essentially unchanged. With the gradually declining cost of training samples, the cost of prediction samples would lower and lower. Then we can get much better solution, which spectrum has same accuracy and its cost much lower than classical network.

3. Results and discussion

Our Guide-Resnet could generate multilayer films with high accuracy. 1000 additional samples are generated as the testing set, and they have random thicknesses and random kinds of metal, which are different from the training set. The average relative error of spectrum is less than 5%. More importantly, the cost of predicted structure is much lower than the network without guiding mechanism. For example, table 1 lists the target and prediction results of an 10-layer film. The “Target” column lists the structure parameters needed by user. The central column lists the result predicted by CNN without guiding mechanism. The right column lists the result predicted by CNN with guiding mechanism. The key difference is in layer 5. With guiding mechanism, the learned model replaces the expensive Au by cheaper Cu. So the cost is only 3.3% of target device. Without guiding mechanism, the cost of predicted structure is 135.9% of target device.

### Table 1 prediction results of an nanocomposite film with 10 layers

| Layer | Target   | Prediction by Resnet | Prediction by Guide-Resnet |
|-------|----------|----------------------|---------------------------|
| 1     | Al - 5nm | Al - 7nm             | Al - 5nm                  |
| 2     | SiO2 – 7nm | SiO2 – 9nm         | SiO2 – 9nm                |
|   |     |     |     |
|---|-----|-----|-----|
| 3 | Ag  | Ag  | Ag  |
|   | 6nm | 8nm | 5nm |
| 4 | SiO2| SiO2| SiO2|
|   | 11nm| 20nm| 14nm|
| 5 | Au  | Au  | Cu  |
|   | 6nm | 8nm | 5nm |
| 6 | SiO2| SiO2| SiO2|
|   | 8nm | 14nm| 18nm|
| 7 | Ag  | Ag  | Ag  |
|   | 8nm | 8nm | 5nm |
| 8 | SiO2| SiO2| SiO2|
|   | 32nm| 19nm| 19nm|
| 9 | Al  | Al  | Al  |
|   | 9nm | 7nm | 5nm |
| 10| SiO2| SiO2| SiO2|
|   | 37nm| 35nm| 32nm|
| relative cost | 135.9% | 3.3% |

Figure 3 compares the spectrum of target and prediction without guiding mechanism. Figure 4 compares the spectrum of target and prediction with guiding mechanism. We can see both predictions have high accuracy. So our guiding mechanism enhanced network could predict structures with both high accuracy and low cost.

![Figure 3](image1)

Figure 3. The left figure showes the target(user-need spectrums). The middle figure showes the predicted spectrums by Resnet. The right figure showes the difference between target and predict result.

![Figure 4](image2)

Figure 4. The left figure showes the target(user-need spectrums). The middle figure showes the predicted spectrums by Guide-Resnet. The right figure showes the difference between target and predict result.

### 4 Conclusions

We present a novel guiding mechanism for the inverse design of SPP devices. Comparing with user requirements, the average relative error of spectrum is less than 5%. More importantly, the cost of predicted structure is much lower than standard deep CNN. This approach is the fist step to find the optimal solution and can be extended to many other inverse design problems in nanophotonics.
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