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INVERSE DESIGN OF METASURFACE BASED ON NEURAL NETWORK

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Abstract

As a kind of artificial electromagnetic interface, optical metasurface performs well in the manipulation and control of the beam. The inverse design of the characteristic parameters based on the objective can be applied to the design of the metasurface structure through the combination of artificial intelligence algorithm and numerical simulation. It presets the structure shape of the metasurface according to the optimization target, determines the parameter to be optimized and its value range, and then selects the appropriate optimization algorithm for optimization, including genetic algorithm, gradient descent algorithm, and density penalty algorithm, etc. According to the objective of optimization, the objective function is written, and the required parameters are optimized.

1 Introduction

As a kind of artificial material, metasurface has attracted much attention due to its flexible optical operation over subwavelength propagation distance [1-3]. It consists of a series of planar artificial units arranged and combined in a specific order. Based on Huygens principle, the artificial units in different areas of the plane are precisely designed to obtain the metasurface with various electromagnetic wave reflection or transmission phase distribution, which can realize the high efficient control of electromagnetic wave[4,5].

The traditional design is to accurately predict the spectral properties and functions of the metasurface by applying iterative calculation scheme combined with FEM [6,7] or FDTD[8,9], and then prepare the metasurface nanostructures according to the model. A set of discrete elements is obtained by calculating the phase amplitude variation of the radiation field in the whole parameter space. For FDTD, the process of TDTD is as follows: the differential expression in Maxwell's domain field curl equation is replaced by the finite difference expression, so as to obtain the finite difference expression of the field components. For the object under study, we can use the same grid of electrical parameters for simulation, select a reasonable initial value of the field and the boundary conditions of the calculation space for calculating, obtain the numerical solution of Maxwell's equations with time factor, and obtain the frequency domain solution in the three-dimensional space through Fourier transform. The motion law and process of electromagnetic wave in electromagnetic field are simulated by computer [10]. However, the calculation and design process of traditional design methods are complicated and time-consuming. Moreover, the shape of the designed metasurface is relatively regular, and the ability to control the beam is also limited.

The main work is to realize the inverse design of the metasurface by training a deep neural network and realize beamforming. Unlike most works, which relying on the training set of known devices, the core idea of this paper is directly learning the physical relationship between device geometry and response through electromagnetic simulations. Then, the trained network will promptly calculate the requirements of the target and output a metasurface structure that matches the expected target.

2 Method

In the one-dimensional case, the EM wave propagates along the z-axis, and the medium parameters and field quantities are independent of x, y, $\partial/\partial x = 0$, $\partial/\partial y = 0$, so Maxwell's equation[11] is

$$-\frac{\partial H_y}{\partial z} = \varepsilon \frac{\partial E_x}{\partial t} + \sigma E_x \tag{1}$$

$$\frac{\partial E_x}{\partial z} = -\mu \frac{\partial H_y}{\partial t} - \sigma_m H_y \tag{2}$$

Sampling of E and H component space nodes in one-dimensional case is shown in the figure.

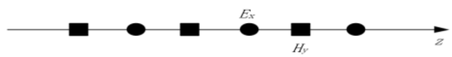

***Figure 1** Sampling of E and H component space nodes in one-dimensional case.*

The FDTD dispersion of equation (1-2) are

$$E_x^{n+1}(k) = CA(m) \cdot E_x^{n}(k) - CB(m) \cdot \left[\frac{H_y^{n+\frac{1}{2}}\left(k+\frac{1}{2}\right) - H_y^{n+\frac{1}{2}}\left(k-\frac{1}{2}\right)}{\Delta z} \right] \tag{3}$$

$$H_y^{n+\frac{1}{2}}\left(k+\frac{1}{2}\right)=CP(m)\cdot H_y^{n-\frac{1}{2}}\left(k+\frac{1}{2}\right)-CQ(m)\cdot\left[\frac{E_x^n(k+1)-E_x^n(k)}{\Delta z}\right] \tag{4}$$

Among them, CA, CB, CP, CQ are respectively

$$CA(m)=\frac{\frac{\varepsilon(m)}{\Delta t}-\frac{\sigma(m)}{2}}{\frac{\varepsilon(m)}{\Delta t}+\frac{\sigma(m)}{2}}=\frac{1-\frac{\sigma(m)\Delta t}{2\varepsilon(m)}}{1+\frac{\sigma(m)\Delta t}{2\varepsilon(m)}}$$

$$CB(m)=\frac{1}{\frac{\varepsilon(m)}{\Delta t}+\frac{\sigma(m)}{2}}=\frac{\frac{\Delta t}{\varepsilon(m)}}{1+\frac{\sigma(m)\Delta t}{2\varepsilon(m)}} \tag{5}$$

$$CP(m)=\frac{\frac{\mu(m)}{\Delta t}-\frac{\sigma_m(m)}{2}}{\frac{\mu(m)}{\Delta t}+\frac{\sigma_m(m)}{2}}=\frac{1-\frac{\sigma_m(m)\Delta t}{2\mu(m)}}{1+\frac{\sigma_m(m)\Delta t}{2\mu(m)}}$$

$$CQ(m)=\frac{1}{\frac{\mu(m)}{\Delta t}+\frac{\sigma_m(m)}{2}}=\frac{\frac{\Delta t}{\mu(m)}}{1+\frac{\sigma_m(m)\Delta t}{2\mu(m)}}$$

where m represents a set of integers or half-integers at the observation point (x,y,z).

For functions defined in the discrete domain, convolution is defined as

$$(f*g)[m]=\sum_n f[n]g[m-n] \tag{5}$$

In a convolutional neural network[12-15], if the input size is set as (N,C_{in},H,W), the output size is $(N,C_{out},H_{out},W_{out})$, then the mathematical expression of the convolutional layer is

$$out(N_i,C_{out_j})=bias(C_{out_j})+\sum_{k=0}^{C_{in}-1} weight(C_{out_j},k)*input(N_i,k) \tag{6}$$

where input and out represent the input and output data of the current convolutional layer respectively. Weight and bias represent the current volume respectively the weight parameters and bias parameters of the layer.

Ignore the bias, the padding is 1, the size of the convolution kernel is 3×3, and the calculation formula of the output coordinate point (i,j) of the convolution layer is

$$out_{i,j}=\sum_{m=i-1}^{i+1}\sum_{n=j-1}^{j+1} weight_{m-i+1,n-j+1}input_{m,n} \tag{7}$$

In the one-dimensional case,

$$out_i=\sum_{m=i-1}^{i+1} weight_{m-i+1}input_m \tag{8}$$

We can change the value of W to achieve forward or backward differentiation. In the one-dimensional case, when the corresponding parameters of the convolution kernel are the same as the difference, the difference can be regarded as a special convolution, and the mathematical equivalence relationship makes it possible to use the convolution instead of the difference to implement the FDTD method. This also provides a theoretical basis for the neural network to directly learn the physical relationship between device geometry and response through electromagnetic simulation during the design of metasurface.

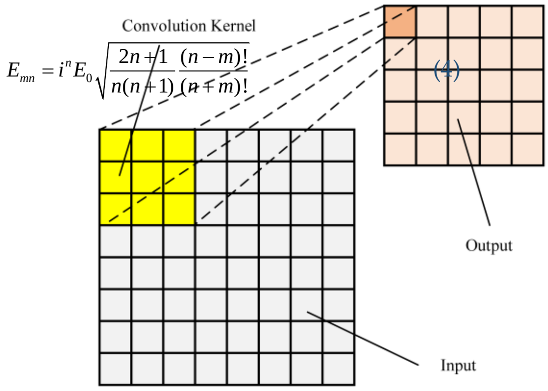

***Figure 2** Convolution operation.*

3 Discussion and conclusion

In this work, in the design process of using neural network to realize metasurface, we realize the inverse design of metasurface by directly learning the physical relationship between device geometry and response by combining electromagnetic simulation, in order to avoid the preparation of large data sets, to realize the purpose of beamforming.

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5 References

[1] Yu, Nanfang, Capasso, et al. Flat optics with designer metasurfaces.[J]. Nature Materials, 2014.

[2] Yu N , Aieta F , Genevet P , et al. A broadband, background-free quarter-wave plate based on plasmonic metasurfaces.[J]. Nano Letters, 2012, 12(12):6328-6333.

[3] Zhao Y , Alu A . Tailoring the dispersion of plasmonic nanorods to realize broadband optical meta-waveplates.[J]. Nano Letters, 2013, 13(3):1086-1091.

[4] Kildishev A V , Boltasseva A , Shalaev V M . Planar Photonics with Metasurfaces[J]. Science, 2013, 339(6125):1232009.

[5] Light Propagation with Phase Discontinuities: Generalized Laws of Reflection and Refraction.[J]. Science, 2011.

[6] Noguchi S , Matsutomo S , Cingoski V . An Adaptive FEM Based on Magnetic Field Conservation Applying to Ferromagnetic Problems[J]. IEEE Transactions on Magnetics, 2018, PP(3):1-4.

[7] Zhang R , Jia P , Hu L , et al. FEM-DDM-BEM for a 3-D Electromagnetic Scattering Analysis of Metal Dieletric Composite Structure[C]// International Conference on Computational Electromagnetics. 0.

[8] Yee K S . Numerical solution of initial boundary value problems involving maxwell's equations in isotropic media[J]. IEEE Transactions on Antennas & Propagation, 1966, 14(5):302-307.

[9] Ohtani T , Kanai Y , Kantartzis N V . Wide-angle elimination of TF/SF-generated spurious waves in the nonstandard-FDTD technique[C]// Electromagnetic Field Computation. IEEE, 2016.

[10] Kasher J C, Yee K S. A numerical example of a two-dimensional scattering problem using a subgrid[J]. Applied Compzrtational Electromagnetics Society Journal and Newsletter, 2, 1987, 2: 75-102.

[11] TAFLOVE A, HAGNESS S. Computational electrodynamics: the finite-difference time-domain method[J]. Optical Technology, 2005, 5(15):629-670.

[12] KRIZHEVSKY, ALEX, SUTSKEVER, ILYA, HINTON, GEOFFREY E.. ImageNet Classification with Deep Convolutional Neural Networks[J]. Communications of the ACM,2017,60(6):84-90. DOI:10.1145/3065386.

[13] He M Y , Li J J . Machine Learning Based Neural Network Solving Methods for the FDTD Method[C]// 2018 IEEE International Symposium on Antennas and Propagation & USNC/URSI National Radio Science Meeting. IEEE, 2018.

[14] Massa A , Marcantonio D , X Chen, et al. DNNs as Applied to Electromagnetics, Antennas, and Propagation - A Review[J]. IEEE Antennas and Wireless Propagation Letters, 2019, PP(99):1-1.

[15] Ren Y, Dang X, Wang C, et al. Fast RCS Data Generation Based on InfoGAN[C]//2021 Photonics & Electromagnetics Research Symposium (PIERS). IEEE, 2021: 331-336.