Meta-Grating Spectral Beam Deflector with Topology Optimization and Stochastic Gradient Descent Algorithm

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Abstract—This report presents a novel approach for designing a meta-grating spectral beam deflector with unitary amplitude wavelength-independent first-order diffraction. The design process combines the regular adjoint simulation assisted topology optimization with a stochastic gradient descent (SGD) algorithm to overcome the challenge of local optimum pitfall and approach the global optimum solution. The meta-grating geometry is iteratively optimized to achieve the desired diffraction characteristics. The SGD algorithm enables the incorporation of more measurement data and improved optimization convergence. The proposed method demonstrates promising results in achieving the targeted optical performance, showcasing its potential for advanced optical device design.

Index Terms—Topology Optimization, Meta-Grating, Stochastic Gradient Descent

1 Introduction

Metasurfaces are artificially designed thin planner structures with sub-wavelength fine features. It has become the hotspot of research in the field of optics and photonics, due to its remarkable ability to interact with and manipulate the properties of light, including the phase, amplitude, and polarization. By judiciously designing the sub-wavelength features, metasurfaces can fulfill various desired optical functionalities, for instance, beam steering, focusing, holography, and amplitude controlling.

The conventional metasurfaces designing process involves using human intuition and simplified theoretical models, which has been proven to be efficient for simple figures of merit, for instance, transmission efficiency at a single wavelength. However, as the complexity increases, traditional methodologies become increasingly challenging and often result in suboptimal performances. This limitation has paved the way for the development of the inverse design scheme of metasurfaces design, which has gained great interest in recent years [1].

The inverse design of metasurfaces refers to searching for the optimal geometrical structures of the meta-atom components that can yield a desirable optical performance. Previous research has studied diverse optimization algorithms, including topology optimization, genetic algorithms, and machine learning models. Machine learning and generative AI can be extremely powerful in metasurface design [2], [3]. Especially, the large model can be extremely strong at bridging up the complex and hidden relation between the geometrical structure of meta-elements and the output optical performance. However, it requires a large dataset of different metasurface geometries and their corresponding optical response for training purposes. Besides, the computational power consumption can be extremely huge. It opens up a bright future only if these two preconditions are satisfied. Another candidate, genetic algorithms, utilizes completely

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different approaches. Genetic algorithms [4], [5], inspired by biological evolution, mimic the natural evolution process by iteratively modifying a population of candidate metasurface structural solutions. In each iteration, the fittest candidate solutions are selected for reproduction via crossover and mutation operations. Despite the decent performances, the genetic algorithm is again heavily relied on computational resources. In addition, it can suffer from a slow convergence speed.

On the other hand, topology optimization is a lightweight algorithm with a fast convergence [6], [7]. Topology optimization refers to optimizing the material distribution to approach the desired performance. It initiates by pixelating the material distribution inside a design domain, and then iteratively updates the distribution based on the gradient information calculated from electromagnetic simulations. Combining with the adjoint method, the gradient associated with the electromagnetic solver can be directly extracted with the aid of one extra adjoint simulation. This paradigm opens the pathway for efficient metasurface optimization with a fast convergence time. Despite the advantages, solving the electromagnetic problem is still in general time-consuming. Another inherent problem is that the optimization process can be easily trapped by the local optimum, failing to reach the global optimal solution. This issue is especially pronounced for metasurface design due to its highly non-convex nature.

In this report, the objective is to explore the possibility of implementing the stochastic process in a topology optimization algorithm, aiming to develop better robustness against local optimum pitfalls. Specifically here, global optimization is made possible by incorporating stochastic gradient descent in regular topology optimization package. The design problem chosen here is to design for a metagrating structure to achieve visible wavelength-independent unitary first-order diffraction. Designing for a specific spectral behavior is challenging due to the requirements of precise positioning of multiple optical resonances in the wavelength domain. Here the optimal design is automatically searched for based on the gradient information in each iteration. The resulting metagrating can find useful application in lightweight spectroscopy devices or wavelength-dependent beam deflectors, with input light at different wavelengths being deflected into different output angles.

2 Related Work

The previous attempts of incorporating stochastic processes into metasurfaces inverse design are mainly by genetic algorithm approaches [4], [5], [8], where the randomness comes from three parts: 1. The randomly generated initial candidate solutions; 2. New candidate solutions are generated by randomly mutating and recombining (crossover) the selected solutions from the previous generation. 3. The selection process is probabilistic. As a completely different approach using topology optimization, each step is deterministically following the gradient direction. Therefore there is hardly room for stochastic process to come in. Here in this project, the author reports on the attempt to incorporate stochastic gradient descent process into regular topology optimization package to help improve the robustness against local optima.

3 Proposed Method

In this section, the generic topology optimization algorithm is introduced, together with the stochastic gradient descent processes implemented. The topology optimization scheme involved in this report closely follows the approach in Ref. [9].

3.1 Generic Topology Optimization with Adjoint Simulation

In this project, the metasurface topology optimization is carried out on the electromagnetic solver named RETICOLO [10], developed on Matlab. RETICOLO [10] is a semi-analytical method based on rigorous coupled wave analysis, which enables rapid computation of electromagnetic response of periodic planar structures. In specific, the material distribution within one unit cell, which serves as the

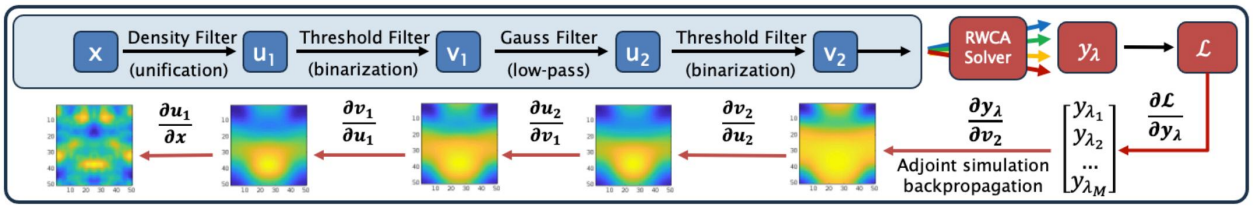

Fig. 1. The topology optimization pipeline. Starting from the inital unit cell geometry x, a series of filters are applied to ensure a few physical and fabrication constraints. In particular, the density filter and Gauss blur filter are for the reduction of excessively small structures and the threshold filters are for the binarization. The resulting pattern v_2 is fed into the RCWA electromagnetic solver to obtain the desired spectrum vector y_λ, which is used to evaluate the final loss function $\mathcal{L}$. The gradients of each step are evaluatable to enable backpropagation and gradient descent.

design space, is specified, and the corresponding electromagnetic behaviors are solved based on scattering matrix formulation.

To make it compatible with topology optimization, the design space inside the unit cell is discretized into fine pixels. Each pixel can take up different values, where "0" and "1" represent absence and presence of material at the specific pixel. To make the geometry differentiable, the allowed value is extended to be continuous in the range between 0 and 1. Each value corresponds an intermediate interpolation between the design material and the background material (usually air). To make the design compatible with realistic material properties, the topology optimization process incorporates binary filter along the iterations. which gradually pushes the value assigned to each pixel to 0 or 1.

Therefore, after specifying several hyperparameters of the unit cell including the periodicity, thickness, and grid sizes, the design object is no different than a gray scale image. On top of that, several useful image processing procedures can be applied onto the image, fulfilling physical constraints or assisting the optimization. For instance, the Gaussian blur filters are used to gradually filter out the excessively fine structures that can result in difficulties in actual fabrication processes. The pipeline used in the topology optimization can be found in Fig.1.

3.1.1 Topology Optimization Pipeline

Starting from an arbitrarily generated pattern "x" as the initial step, a series of filters are applied onto it to enforce physical or fabrication constraints. This includes two threshold filters for binarization purpose, and two blur filters for eliminating excessively small and separate structures. After obtaining the post-filtering pattern v_2, it is fed into the RCWA electromagnetic solver to extract the first-order diffraction spectrum. The spectral information is stored into a vector y_λ. The length of y_λ: M is determined by the number of sampling point in the desired spectrum. A larger M value means much finer spectral feature, which in turn is more difficult to be fit. Finally, the spectrum is compared to the ground truth $\hat{y}$, which is the target spectrum. In this case $\vec{y_i} = 1$. The loss function is the L2 norm distance defined as $\mathcal{L} = ||y_\lambda - \hat{y}||_2^2$.

3.1.2 Adjoint Simulation

In general case, the efficiency to evaluate the gradient associated with electromagnetic problems are low due to the heaviness of electromagnetic simulation itself. For example, for an optimization process with N design parameters, one needs to solve for the Maxwell's equations on the order of N times to obtain the full derivative according to finite difference, and each could cost several minutes time and extensive computational resources. This is especially critical in topology optimization since the volume of the design space can be easily as large as 10^4 or even more.

To resolve the difficulty in electromagnetic calculation, the method of adjoint calculation is employed [62, 63, 64, 65]. Briefly speaking, it

utilizes additional constraints inside the electromagnetic problems to avoid evaluating certain computationally heavy terms and replace it by computationally cheap ones. The key is based on the reciprocity theorem in electromagnetics, where the positions of the source and the generated electric field are interchangeable. Making use of such property, the derivative of certain high-level function $\mathcal{F}$ to the electric field $\mathbf{E}$ can be related to the adjoint field $\mathbf{E}^\dagger$, which can be acquired by measuring the total field response when excited by adjoint field source. For the interest of this project with structure given as a periodic planar geometry, the adjoint field source is the backward incident plane wave. Therefore, the gradient of transmission coefficient over the design space material distribution is given by:

$$\nabla_{v_2} t = \mathcal{N} \iiint \mathbf{E} \cdot \mathbf{E}^\dagger dV, \tag{1}$$

where the overlap integral is evaluated within the unit cell, and $\mathcal{N}$ is the normalization factor. The transmission efficiency is the modulus square of the complex transmission coefficient, therefore the corresponding gradient: $\nabla_{v_2} y = 2\mathcal{R}e\{t \cdot \nabla_{v_2} t\}$.

The resulting spectrum is recorded into a form of vector $y_\lambda = \begin{pmatrix} y_{\lambda_1} \\ y_{\lambda_2} \\ \vdots \\ y_{\lambda_M} \end{pmatrix}$. The loss function is ensembled as the L2 norm between the calculated spectrum and the ground truth: $\mathcal{L} = ||y_\lambda - \hat{y}||_2^2 = \sum_{j=1}^{M} (y_{\lambda_j} - 1)^2$. Therefore the gradient w.r.t. the loss function is of the form:

$$\frac{\partial \mathcal{L}}{y_\lambda} = 2(y_\lambda - \hat{y}).$$

3.1.3 Implementing Stochastic Gradient Descent

One direct way of implementing stochastic processes into the optimization algorithm is at the final step. In particular, during each iteration, p (patch size) random elements are selected from the spectrum vector y_λ. In another word, this is essentially to ask the algorithm to optimize for a better performance based on the gradient information of a random subregion of the spectrum. In the usual case where one puts the full spectrum requirement into the optimizer, each iteration takes a long time by evaluating for all the wavelength sampling points. In addition, due to the spectral correlation (i.e., the transmission at wavelength λ_1 is not independent with transmission at λ_2), using the full gradient information from all the wavelength sampling points can be inefficient when some of the terms counter-interacting with each others. Also, the randomness brought in by the stochastic selection process, to some extent, can avoid the local optimum pitfall and approach the global optimal solution.

4 Experimental Results

4.1 Without Threshold filter

First, a few proof-of-concept attempts are presented to demonstrate the working principle of such optimization scheme. In this part, the threshold filter is turned off for better convergence. The resulting structure will be a distribution of material with interpolated index of refraction from device material (silicon $n = 3.45$ to air $n = 1$). The substrate material is set to silicon dioxide ($n = 1.45$). To obtain the best performance, one has to optimize for a few hyper-parameters first, which includes the layer thickness, the grating periodicity, and the stochastic patch number.

4.1.1 Fitting v.s. Grating Thickness

First, the first-order diffraction spectra are tested with different grating thicknesses. The resulting convergence plots and the corresponding spectra are presented in Fig.2. The optimal thickness from testing is given as 325 nm to 425 nm, resulting in high-transmission efficiency diffraction spectra with near uniform landscape. Here I will use 425 nm in the rest of the report.

4.1.2 Fitting v.s. Grating Periodicity

Then, the first-order diffraction performances are tested on different unit cell periodicities.

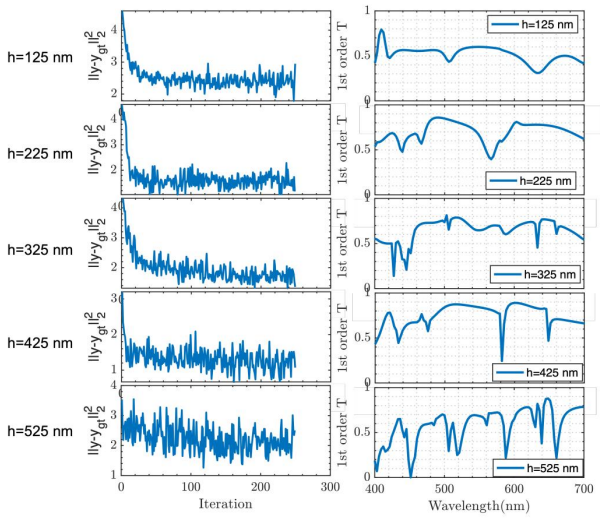

Fig. 2. Test on the optimal grating thickness for wavelength-independent unitary first-order transmission spectra. As compared between different thickness values, the optimal is around 325 to 425 nm.

The pitch value also determines the output angle of the device, therefore it is a critical parameter for practical applications. The results are shown in Fig.3., where the optimal periodicity is determined around $\Lambda = 800nm$.

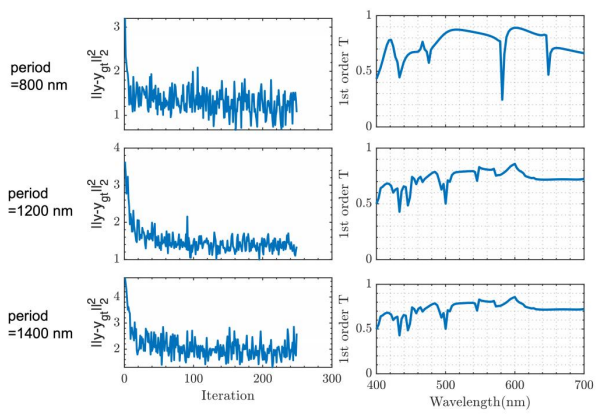

Fig. 3. Test on the optimal grating pitch for wavelength-independent unitary first-order transmission spectra. As compared between different thickness values, the optimal is around 800 nm.

4.2 With Threshold filter

For testing against the stochastic patch sizes, I turned on the threshold filter to simulate situations closer to practical scenarios. The results are presented in Fig.4.

From the result, the best performance is achieved at around patch size = 5, with a nearly uniform first-order diffraction spectrum. Compared to the regular gradient descent algorithm, this is a significant improvement as it cannot reach such a solution, even though taking an excessively long time on a personal PC.

Beyond that, it is surprising to find that the optimal performance is found at around patch size $= 5$. For smaller patch sizes, the convergence behaves poorly due to the random process involved. While for larger patch sizes, there is a general trend with the loss function bouncing back to a larger value. This is never observed when the binarization is turned off. So as the iteration number goes larger, the binarization becomes more drastically and counter-interact with the optimization gradient to further push up the transmission efficiencies. Therefore, a trade-off between the ultimate performance and practical constraint is recognized here.

By further inspection of the performances, the results using intermediate patch sizes (5 or 10) are relatively well-behaved, with a transmission spectrum with broadband high-transmission behavior. Correspondingly, the grating cross-section profiles are different than other low-performance ones as well, with a larger number of grating ridges inside one periodicity. This type of structure with a larger number of ridges is only enabled by appropriately choosing the patch size, where such a trend can open up new findings related to fundamental behaviors of light-matter interaction by inspecting the electric field distribution inside the grating layer.

By comparing to the usual gradient descent algorithm, such a novel algorithm can indeed circumvent the local optimum pitfall by repeatedly resulting in lower loss function states. However, the reflection is that the patch size of the stochastic process has to be carefully chosen as it can determine the degree of deterministic (the location between fully stochastic and fully gradient-determined).

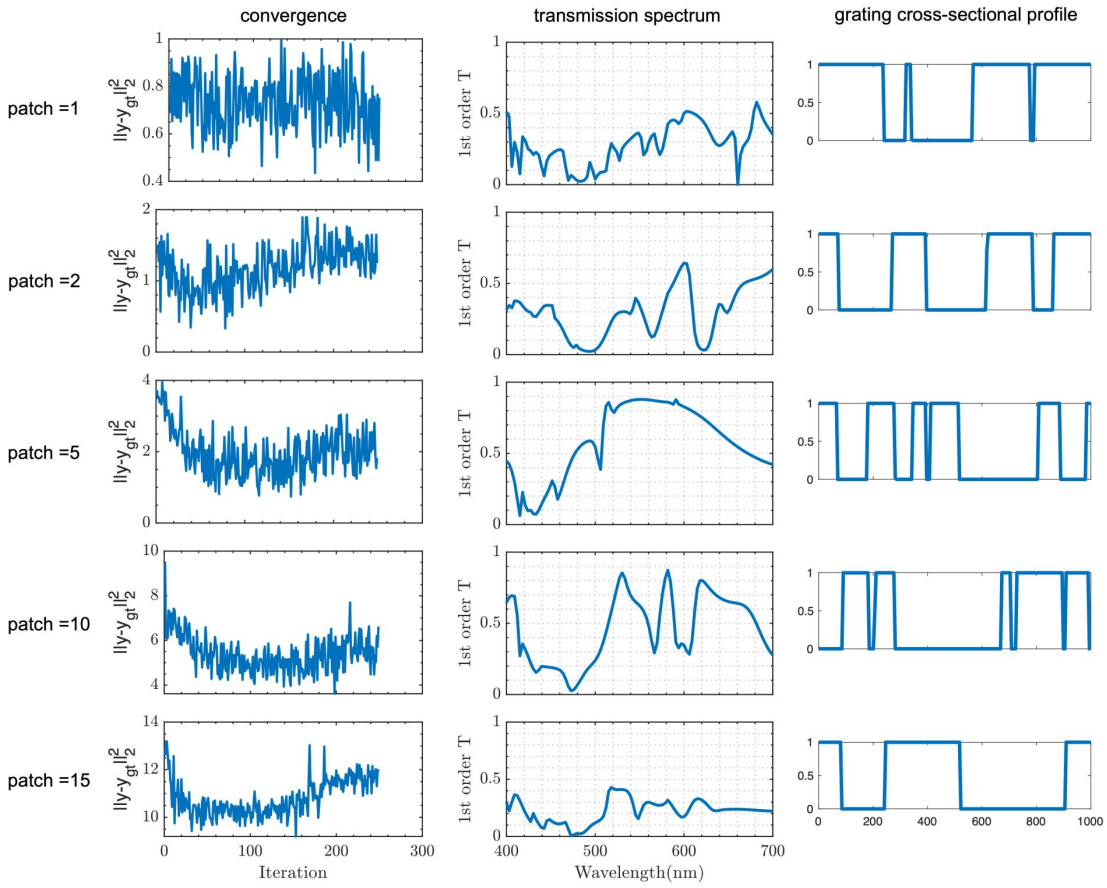

Fig. 4. Test on different stochastic patch sizes for wavelength-independent unitary first-order transmission spectra with the binarization function turned on. The hyperparameters are set to: $\Lambda = 1200nm, h = 425nm$. The optimal patch size is found to be around 5.

5 Conclusions and Outlooks

In this project, a simple stochastic gradient descent process is successfully incorporated into the conventional topology optimization, and its performance is tested by designing a metal-grating with a near-unitary first-order diffraction spectrum. The algorithm with the use of stochastic gradient descent can more easily reach a better optimum point compared to conventional topology optimization algorithms with a gradient descent updating scheme. The optimal solution is found to be as: grating period $\Lambda = 1200nm$, thickness $h = 425nm$, and stochastic patch size around 5 with a silicon 1D-grating on silica substrate configuration. Such an optimization algorithm package can be extended in general to be applied to any spectral design tasks.

The future direction might involve research on possible image processing procedures to decouple the binarization process with the degradation of performances. One possible method would involve remove the binarization filter and add an additional constraint or image prior onto the final loss function to softly enforce binarization.

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