Dataless training of generative models for the inverse design of metasurfaces

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Abstract

Metasurfaces are subwavelength-structured artificial media that can shape and localize electromagnetic waves in unique ways. The inverse design of metasurfaces is a non-convex optimization problem in a high dimensional space, making global optimization a huge challenge. We present a new type of global optimization algorithm, based on the training of a generative neural network without a training set, which can produce high-performance metasurfaces. Instead of directly optimizing devices one at a time, we reframe the optimization as the training of a generator that iteratively enhances the probability of generating high-performance devices. The loss function used for backpropagation is defined as a function of generated patterns and their efficiency gradients, which are calculated by the adjoint variable method using the forward and adjoint electromagnetic simulations. We observe that distributions of devices generated by the network continuously shift towards high-performance design space regions over the course of optimization. Upon training completion, the best-generated devices have efficiencies comparable to or exceeding the best devices designed using standard topology optimization. We envision that our proposed global optimization algorithm generally applies to other gradient-based optimization problems in optics, mechanics and electronics.

1 Introduction

Photonic technologies serve to manipulate, guide, and filter electromagnetic waves propagating in free space and in waveguides. Due to the strong dependence between geometry and function, much emphasis in the field has been placed in identifying geometric designs for these devices given a desired optical response. The vast majority of these design concepts utilize relatively simple shapes that can be described using physically intuition. As examples, silicon photonic devices typically utilize adiabatic tapers and ring resonators to route and filter guided waves [1], and metasurfaces, which are diffractive optical components used for wavefront engineering, typically utilize arrays of nanowaveguides or nanoresonators comprising simple shapes [2]. While these design concepts work well for certain applications, they possess limitations, such as narrow bandwidths and sensitivity to temperature, which prevents the further advancement of these technologies.

To overcome these limitations, design concepts based on optimization have been proposed. Among the most successful of these concepts is the adjoint variables method, which uses gradient descent to iteratively adjust the dielectric composition of the devices and improve device functionality [3-5]. This design method has enabled the realization of high performance, robust [6] devices with nonintuitive layouts, including new classes of on-chip photonic devices with ultrasmall footprints [7], non-linear photonic switches [8], and diffractive optical components that can deflect [9][10] and focus [14] electromagnetic waves with high efficiencies. While adjoint optimization has great potential, it is a local optimizer and depends strongly on the initial distribution of dielectric material in the devices. As such, identifying a high performance device typically requires the optimization of many
devices with random initial dielectric distributions and selecting the best device. This approach is very computationally expensive, preventing the scaling of these concepts to large, multi-functional devices.

We present a new global optimization method that combines adjoint variables electromagnetic calculations with a generative neural network to realize high performance photonic structures. Unlike the adjoint variables method, which optimizes one device at a time, our approach optimizes a distribution of devices, thereby enabling a global search of the design space. As a model system, we will apply our concept to design periodic metasurfaces, or metagratings, which selectively deflect a normal, incident beam to the +1 diffraction order. We emphasize that our proposed concepts are general and apply broadly to design problems in photonics and other fields in the physical sciences in which the adjoint variables method applies.

2 Related Work

In recent years, deep learning has been investigated as a tool to facilitate the inverse design of photonic devices. Initial studies focused on the use of deep neural networks to learn the relationship between device geometry and optical response. When the network is well trained, device geometries can be optimized for a desired optical response using gradients from backpropagation [15–18]. This approach works well on simple device geometries described by a few parameters and possessing a simple optical response. However, the model accuracy decreases as the geometric degrees of freedom increases, making these ideas infeasible for the inverse design of complex systems.

An alternative approach is to utilize generative adversarial networks (GANs) [19], which have been proposed as a tool for freeform device optimization [20, 21]. GANs have been of great interest in recent years and have a broad range applications, including image generation [22, 23], image synthesis [24], image translation [25], and super resolution [26]. In the context of photonics inverse design, GANs are given images of high performance devices as training sets and learn the main geometric features that contribute to high performance. Upon training, they can generate high performance device patterns for parameters different from the training set. GAN-generated devices are good starting points for topology optimization, lead to significant savings in optimization computational time, but they do require a computationally expensive training set. New data-driven concepts that better incorporate physics knowledge into the network training process are required to reduce the need for expensive training data.

3 Problem Setup

![Figure 1: Schematic of a silicon metagrating that deflects normally-incident TM-polarized light of wavelength \( \lambda \) to an outgoing angle \( \theta \). The objective of optimization is to search for the metagrating pattern that maximizes deflection efficiency.](image)

The metagratings consist of silicon nanoridges and deflect normally-incident light to the +1 diffraction order (Figure 1). The thickness of the gratings is fixed to be 325 nm and the incident light is TM-polarized. The refractive index of silicon is taken from Ref. [27] and only the real part of the index is used to simply the design problem. For each period, the metagrating is subdivided into \( N = 256 \)
segments, each possessing a refractive index value between silicon and air during the optimization process. These refractive index values are the design variable in our problem and are specified as $x \in \mathbb{R}^N$. The deflection efficiency is defined as the power of light going into the desired direction of deflection angle $\theta$ normalized to power of incident light. The deflection efficiency is a nonlinear function of index profile $\text{Eff} = \text{Eff}(x)$, governed by Maxwell’s equations. This quantity, together with the electric field profiles within a device, can be accurately solved using a wide range of electromagnetic solvers.

Our optimization objective is to maximize the deflection efficiency of the metagrating at a specific operating wavelength $\lambda$ and outgoing angle $\theta$:

$$x^* := \arg\max_{x \in \{-1,1\}^N} \text{Eff}(x) \quad (1)$$

Here, we are interested in physical devices that possess binary index values in the vector: $x \in \{-1,1\}^N$, where -1 represents air and +1 represents silicon.

4 Methods

Our proposed inverse design scheme is shown in Figure 2. Instead of directly optimizing a single device, which is the case of the adjoint variables method, we optimize a distribution of devices by training a generative neural network. Uniquely, our scheme does not require any pre-prepared training data. The input of the generator is a random noise vector $z \in \mathcal{U}(-a,a)$ and has the same dimension as the output device index profile $x \in [-1,1]^N$. $a$ is the noise amplitude. The generator is parameterized by $\phi$, which relates $z$ to $x$ through a nonlinear mapping: $x = G_\phi(z)$. In other words, the generator maps a uniform distribution of noise vectors to a device distribution $G_\phi : \mathcal{U}^N(-a,a) \mapsto \mathcal{P}_\phi$, where $P_\phi(x)$ defines the probability of $x$ in device space $S = [-1,1]^N$. We frame the objective of the optimization as maximizing the probability of the highest efficiency device in $S$:

$$\phi^* := \arg\max_{\phi} \int_S \delta (\text{Eff}(x) - \text{Eff}_{\text{max}}) \cdot P_\phi(x) \, dx \quad (2)$$

4.1 Loss Function Formulation

While our objective function above is rigorous, it cannot be directly used for network training due to two reasons. The first is that the derivative of the $\delta$ function is nearly always zero. To circumvent this issue, we note that the $\delta$ function can be rewritten as the following:

$$\delta (\text{Eff}(x) - \text{Eff}_{\text{max}}) = \lim_{\sigma \to 0} \frac{1}{\sqrt{\pi \sigma}} \exp \left[ - \left( \frac{\text{Eff}(x) - \text{Eff}_{\text{max}}}{\sigma} \right)^2 \right] \quad (3)$$
By substituting the $\delta$ function with this Gaussian form and leaving $\sigma$ as a tunable parameter, we relax Equation 2 and it becomes:

$$
\phi^* := \arg\max_{\phi} \int_{S} \exp\left[-\left(\frac{\text{Eff}(x) - \text{Eff}_{max}}{\sigma}\right)^2\right] \cdot P_{\phi}(x)dx 
$$

The second reason is that the objective function depends on the maximum of efficiency $\text{Eff}_{max}$, which is unknown. To address this problem, we approximate Equation 4 with a different function, namely the exponential function:

$$
\phi^* := \arg\max_{\phi} \int_{S} \exp\left(\frac{\text{Eff}(x) - \text{Eff}_{max}}{\sigma}\right) \cdot P_{\phi}(x)dx
$$

This approximation works because $P_{\phi}(x \mid \text{Eff}(x) > \text{Eff}_{max}) = 0$ and our new function only needs to approximate that in Equation 4 for efficiency values less than $\text{Eff}_{max}$. With this approximation, we can remove $\text{Eff}_{max}$ from the integral:

$$
\phi^* := \arg\max_{\phi} A \int_{S} \exp\left(\frac{\text{Eff}(x)}{\sigma}\right) \cdot P_{\phi}(x)dx
$$

$A = \exp(-\text{Eff}_{max}/\sigma)$ is the normalization factor and does not affect the optimization. The precise form of the approximation function can vary and be tailored depending on the specific optimization problem. For this study, we will use Equation 6.

In practice, we will be sampling a batch of devices $\{x^{(m)}\}_{m=1}^{M}$ from $P_{\phi}$. We then further approximate the objective function as:

$$
\phi^* := \arg\max_{\phi} \mathbb{E}_{x \sim P_{\phi}} \exp\left(\frac{\text{Eff}(x)}{\sigma}\right)
$$

$$
\approx \arg\max_{\phi} \frac{1}{M} \sum_{m=1}^{M} \exp\left(\frac{\text{Eff}(x^{(m)})}{\sigma}\right) 
$$

We note that the deflection efficiency of device $x$ is calculated using an electromagnetic solver, such that $\text{Eff}(x)$ is not directly differentiable for backpropagation. To bypass this problem, we use the adjoint variables method to compute efficiency gradient with respect to refractive indices for device $x$: $g = \frac{\partial \text{Eff}}{\partial x}$ (Figure 2). Details pertaining to these gradient calculations can be found in other inverse design papers [9, 8, 7]. To summarize, the electric field terms from the forward simulation $E^{fwd}$ are calculated by propagating a normally-incident electromagnetic wave from the substrate to the device, as shown in Figure 1. The electric fields from the adjoint simulation $E^{adj}$ are calculated by propagating an electromagnetic wave in the direction opposite of the desired outgoing direction from the forward simulation. The efficiency gradient $g$ is calculated by integrating the overlap of those electric field terms:

$$
g = \frac{\partial \text{Eff}(x)}{\partial x} \propto \text{Re}(E^{fwd} \cdot E^{adj})
$$

Finally, we use our adjoint gradients and objective function to define the loss function $L = L(x, g)$. Our goal is to define $L$ such that minimizing $L$ is equivalent to maximizing the objective function $\frac{1}{M} \sum_{m=1}^{M} \exp\left(\frac{\text{Eff}(x^{(m)})}{\sigma}\right)$ during generator training. With this definition, $L$ must satisfy $-\frac{\partial L}{\partial x^{(m)}} = \frac{1}{M} \frac{\partial}{\partial x^{(m)}} \exp\left(\frac{\text{Eff}(x^{(m)})}{\sigma}\right)$ and is defined as:

$$
L(x, g) = -\frac{1}{M} \sum_{m=1}^{M} \frac{1}{\sigma} \exp\left(\frac{\text{Eff}(m)}{\sigma}\right) x^{(m)} \cdot g^{(m)}
$$

$\text{Eff}(m)$ and $g^{(m)}$ are independent variables calculated from electromagnetic solver, which are detached from $x^{(m)}$. We also add a regularization term $-|x| \cdot (2 - |x|)$ to $L$ to ensure binarization of the generated patterns. This term reaches a minimum when generated patterns are fully binarized. A coefficient $\gamma$ is introduced to balance binarization with efficiency enhancement in the final loss function:

$$
L(x, g) = -\frac{1}{M} \sum_{m=1}^{M} \frac{1}{\sigma} \exp\left(\frac{\text{Eff}(m)}{\sigma}\right) x^{(m)} \cdot g^{(m)} - \gamma \cdot \frac{1}{M} \sum_{m=1}^{M} |x^{(m)}| \cdot (2 - |x^{(m)}|)
$$
4.2 Network Architecture

The architecture of the generative neural network is adapted from DCGAN [28], which comprises 2 fully connected layers, 4 transposed convolution layers, and a Gaussian filter at the end to eliminate small features. LeakyReLU is used for activation functions except for the last layer, which uses a tanh. We also add dropout layers and batchnorm layers to enhance the diversity of the generated patterns. Periodic paddings are used to account for the fact that the devices are periodic structures.

4.3 Training Procedures

Algorithm 1: Generative neural network-based optimization

Parameters: $a$, noise amplitude. $M_0$, initial batch size. $\sigma$, loss function coefficient. $\alpha$, learning rate. $\beta_1$ and $\beta_2$, momentum coefficients. $\gamma$, binarization coefficient.

initialization;

while $i < \text{Total iterations}$ do

Choose a batch size $M_i$;

Sample $\{z^{(m)}\}_{m=1}^{M_i} \sim \mathcal{U} N(-a, a)$;

$\{x^{(m)} = G_{\phi}(z^{(m)})\}_{m=1}^{M_i}$, device samples;

$\{g^{(m)}\}_{m=1}^{M_i}$, $\{\text{Eff}^{(m)}\}_{m=1}^{M_i}$ ← forward and adjoint simulations;

$g_{\phi} \leftarrow \nabla_{\phi} \left[ \frac{1}{M_i} \sum_{m=1}^{M_i} \frac{1}{\sigma} \exp \left( \frac{\text{Eff}^{(m)}}{\sigma} \right) x^{(m)} \cdot g^{(m)} + \gamma \cdot \frac{1}{M_i} \sum_{m=1}^{M_i} |x^{(m)}| \cdot (2 - |x^{(m)}|) \right]$;

$\phi \leftarrow \phi + \alpha \cdot \text{Adam}(\phi, g_{\phi})$;

end

$x^* \leftarrow \text{argmax}_{x \in \{x^{(m)} | x^{(m)} \sim P_{\phi^*}\}_{m=1}^{M}} \text{Eff}(x)$

The training procedure is shown in Algorithm 1. Initially, the device distribution $P_\phi$ is roughly an uniform distribution over the whole device space $\mathcal{S}$. During the training process, $P_\phi$ is continuously refined and shifted towards the high-efficiency device subspace. When the generator is well trained, the devices produced from the generator have a high probability to be highly efficient. By taking the best device from the optimized device batch $\{x^{(m)} | x^{(m)} \sim P_{\phi^*}\}_{m=1}^{M}$, there is a possibility for the optimizer to get to the global optimum.

Noise amplitude $a$ and batch size $M$ are important hyperparameters in the network training. In order to fully sample the device space $\mathcal{S}$ in the early stage of training, the batch size should initially be relatively large and then gradually reduce to a small number when device samples start to cluster. $a$ should be a relatively large number $\sim 10 - 40$ for Xavier initialization.

4.4 Comparison with brute-force searching

In many inverse design approaches, brute-force searching with local optimizers is used to find out the global optimum. A large number of device patterns are randomly initialized and then optimized individually using gradient descent. The highest efficiency device among those optimized devices is taken as the final design. With this approach, many devices usually get trapped in local optima in $\mathcal{S}$. Additionally, finding the global optimum in a very high dimensional space is more challenging with this method.

In our proposed inverse design scheme, we optimize a distribution of devices. As indicated in Equation (11), higher efficiency devices bias the generator more than low-efficiency devices, which is helpful to avoid low-efficiency local optima. The device distribution dynamically changes during the training process, and over the course of optimization, more calculations are performed to explore more promising parts of the design space and away from low-efficiency local optima.
5 Experiments

5.1 A toy model test

We first perform our algorithm on a simple testing case, where the dimensions of the input $z$ and output $x$ are 2. The "efficiency" function $\text{Eff}(x)$ is defined as:

\[
\text{Eff}(x_1, x_2) = \exp(-2x_1^2) \cos(9x_1) + \exp(-2x_2^2) \cos(9x_2)
\]  

(12)

which is a non-convex function with plenty of local optima and one global optimum at $(0, 0)$. We used Algorithm 1 to search for the global optimum. Hyperparamters are chosen as $\alpha = e^{-3}$, $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\alpha = 30$, and $\sigma = 0.5$, and the batch size $M = 100$ is constant. The generator is trained for 150 iterations and the generated samples over the course of training are shown as red dots in Figure 3. Initially, the samples spread out over the $x$ space, then gradually converge to a cluster located at the global optimum. No samples are trapped in local optima. We repeated the experiments 100 times, and 96 of them successfully found the global optimum.

Figure 3: A toy model test. Samples generated from the generator, shown as red dots, evolve in the $[-1, 1]^2$ space over the course of training.

5.2 Inverse design of metagratings

Finally, we apply our algorithm to the inverse design of 63 different types of metagratings, each with differing operating wavelengths and deflection angles. The wavelengths $\lambda$ range from 800 nm to 1200 nm, in increments of 50 nm, and the deflection angles $\theta$ range from 40 degrees to 70 degrees, in increments of 5 degrees.

Figure 4: (a) Plot of efficiency for devices operating with different wavelength and angle values, designed using brute-force topology optimization. For each wavelength and angle combination, 500 individual topology optimizations are performed and the highest efficiency device is used for the plot. (b) Plot of efficiency for devices designed using generative neural network-based optimization. For each wavelength and angle combination, 500 devices are generated and the highest efficiency device is used for the plot.
The network is implemented using the pytorch-1.0.0 package. The forward simulations and adjoint simulations are performed using the Reticolo RCWA electromagnetic solver in MATLAB. The network is trained on an Nvidia Titan V GPU and 4 CPUs, and it takes 10 minutes for one device optimization. Code implementation can be found at https://github.com/jiaqi65/GLOnet.git

Figure 5: Efficiency histograms of devices designed using brute-force topology optimization (red) and generative neural network-based optimization (blue). The statistics of device efficiencies in each histogram are also displayed. For most wavelength and angle values, the efficiency distributions from generative neural network-based optimization are narrower and have higher maximum values compared to those from brute-force optimization.

5.2.1 Implementation details

The hyperparameters we used are $\alpha = 0.05$, $\beta_1 = 0.9$, $\beta_2 = 0.99$, $\alpha = 40$, $\sigma = 0.2$, and $\gamma = 0.05$. The initial batch size is 500 and gradually decreases to 20. To prevent vanishing gradients when the generated patterns are binarized as $x \in \{-1, 1\}^N$, we replace the last activation function $\tanh$ with $\tanh^2$. For each combination of wavelength and angle, we train the generator for 200 iterations. When the training is done, 500 device samples are produced by the generator and the highest efficiency device is taken as the final design.

The network is implemented using the pytorch-1.0.0 package. The forward simulations and adjoint simulations are performed using the Reticolo RCWA electromagnetic solver in MATLAB. The network is trained on an Nvidia Titan V GPU and 4 CPUs, and it takes 10 minutes for one device optimization. Code implementation can be found at https://github.com/jiaqi65/GLOnet.git
5.2.2 Baseline

We compare our method with brute-force topology optimization. For each design target \((\lambda, \theta)\), we start with 500 random gray-scale vectors, and then iteratively optimize each device using efficiency gradients with respect to device patterns, which are calculated from forward simulation and backward simulation. A threshold filter is used to binarize the device patterns. Each starting point is also optimized for 200 iterations, and the highest efficiency device among 500 candidates is taken as final design.

5.2.3 Results

The efficiencies for devices designed using brute-force optimization and our method are shown in Figure 4. 86% of devices from generative neural network based optimization have higher efficiency than those from brute-force optimization, and on average are 7.2% higher. The efficiency histograms from generative neural network-based optimization and brute-force optimization, for select wavelength and angle pairs, are displayed in Figure 5. For most cases, efficiency histograms produced from our method have higher average efficiencies and maximal efficiencies, indicating that low-efficiency local optima are often avoided during the training of the generator.

6 Conclusions and Future Directions

In this paper, we present a generative neural network-based global optimization algorithm for meta-surface design. Instead of optimizing many devices individually, we reframe the global optimization for this non-convex problem as the training of a generator to generate high efficiency devices with high probability. The efficiency gradients of all device samples collectively improve the performance of the generator, which is helpful to explore the whole device space \(S\) and avoid low-efficiency local optima.

In the future, we are interested in applying our algorithm to more complex systems, such as 2D or 3D metasurfaces, multi-function metasurfaces, and other photonics design problems. A deeper understanding of loss function engineering is necessary for multi-function metasurfaces design, which require optimizing multi-objectives simultaneously. We envision that our algorithm has strong potential to solve inverse design problems in other areas of the physical sciences, such as mechanics and electronics.

References


