Accelerating Inverse Design of Nanostructures Using Manifold Learning

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Abstract

Deep learning and machine learning have recently attracted remarkable attention in the inverse design of nanostructures. However, limited works have used these techniques to reduce the design complexity of structures. In this work, we present an evolutionary-based method using manifold learning for inverse design of nanostructures with minimal design complexity. This method encodes the high dimensional spectral responses obtained by electromagnetic simulation software for a class of nanostructure with different design complexities using an autoencoder (AE). We model the governing distributions of the data in the latent space using Gaussian mixture models (GMM) which then provides the level of feasibility of a desired response for each structure and use a neural network (NN) to find the optimum solution. This method also provides valuable information about the underlying physics of light-matter interactions by representing the sub-manifolds of feasible regions for each design complexity level (i.e., number of design parameters) in the latent space. To show the applicability of the method, we employ this technique for inverse design of a class of nanostructures consisting of dielectric metasurfaces with different complexity degrees.

1 Introduction

Many researchers have conducted extensive research on inverse design of nanophotonic structures due to their unique features in manipulating light in sub-wavelength regime with applications in signal processing [1], image processing [2], lens design [3], bio sensing [4], computing[5], reconfigurable metasurfaces [6], microresonators [7], etc. Deep learning (DL) and machine learning (ML) techniques are recently superseding the conventional approaches for design of nanostructures (e.g., genetic algorithm, exhaustive search, topology optimization, etc.) due to their capability in extracting features from high dimensional data and accelerating the inverse design [8–10]. However, few works address the application of ML and DL for understanding the underlying physics of these structures. In a more intelligent setting, DL has been used for knowledge discovery and this knowledge in turn will be used to accelerate the design process [11–21]. With advances in computational power and distributed DL platforms [22], most of the works do not leverage the intelligence aspect of artificial intelligence (AI), and a large portion of this vast power is wasted for unnecessary complexities in the structures. The current methods are mainly based on the combination of employing neural networks (NN) and a cyclic search. Even though this combination can reduce the complexity of the design problem, a good

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portion of computation is still invested in the cyclic search part [23]. This necessitates the urgency of providing an intelligent approach to address the aforementioned issues.

In this paper, we present a new approach based on manifold learning [24–26] to accelerate designing of nanophotonic structures for achieving a desired response (i.e., reflection spectra of light in a certain bandwidth). The technique finds the desired nanostructures with minimal fabrication complexity by evolving from an initial design to the least complex nanostructure. In addition to reducing the design complexity, this approach provides priceless information about the underlying physics of nanostructures through visualization of the responses in the latent space.

2 Method

The forward problem in designing nanophotonic structures is finding the response for a set of input design parameters. We consider this as the mapping $\mathcal{F}: \mathcal{X} \to \mathcal{Y}$, where $\mathbf{x} \in \mathcal{X}$ is a vector of design parameters and $\mathbf{y} \in \mathcal{Y}$ is the corresponding response. Electromagnetic (EM) simulation softwares like COMSOL Multiphysics, CST Microwave Studio, Lumerical, etc. are the common tools for solving the forward problem in the nanophotonics society. However, the goal of inverse problem is to find the set of design parameters that results in the desired response, and we consider this unknown relation as the mapping $\mathcal{G}: \mathcal{Y} \to \mathcal{X}$. In other words, we seek to find $\mathbf{x}$ such that $\mathbf{x} = \mathcal{G}(\mathbf{y}^*)$. Evaluating $\mathcal{G}$ is not possible as we don't have access to $\mathcal{G}$. So we formulate this problem in terms of $\mathcal{F}$, which is available for us, within an optimization framework:

$$\mathbf{x}^* = \underset{\mathbf{x} \in \mathcal{X}}{\arg\min} \quad Loss(\mathbf{y}, \mathbf{y}^*) \tag{1}$$

where $\mathbf{y} = \mathcal{F}(\mathbf{x})$, $\mathbf{y}^* = \mathcal{F}(\mathbf{x}^*)$, and $Loss$ can be any of the available loss functions that suit the problem (e.g. mean squared error (MSE)). This problem does not have a closed form formulation due to the complexity of the input to output relation in nanophotonic structures and also suffers from non-convexity and non-uniqueness challenge (i.e., for a desired response, there might be multiple sets of design parameters) [16]. The current methods for solving inverse problems in nanophotonics are based on brute-force search methods for finding the vector $\mathbf{x}_i$ that results in the minimal MSE (i.e., $||\mathbf{y}_i - \mathbf{y}^*||_2^2$) or limit themselves to a certain part of the design space and model the inverse mapping to find the local minimum solution [27–29]. However, these methods do not consider the design complexity of the structure in solving the inverse problem and converge to a highly complex structure, while a coarser structure has the ability to produce comparable results. In this research, we use a manifold learning-based method to form the feasible set of responses for each design complexity in the latent space $\mathcal{Z}$ for a class of nanostructures, and solve the inverse problem with the minimal design complexity. To show the capability of our method, we apply this approach to inverse design of a class of nanostructure with different design complexities. Figure 1 shows the unit cell of the nanostructures, consisting of one to four ellipsoids of HfO_2 on the top of SiO_2 substrate [30]. As shown in Fig. 1, the number of design parameters and complexity of the structure increases as we add more ellipsoids. For each structure, we randomly generate a set of design parameters and find the corresponding reflection responses using EM software (i.e., Lumerical). Then we train an AE to reduce the dimensionality of the response space $\mathcal{Y}$. To model the distribution of the manifold of feasible responses for each structure, we use GMM [31]. Finally, we train a NN from the design to the response space and use that to find the set of design parameters for a desired response.

The first step in our design approach, is learning the manifold of the responses in the latent space by reducing the dimensionality of the response space. A popular and efficient approach for non-linear dimensionality reduction (DR) is using AE [32]. AEs are artificial NNs which have the same input and output and a bottleneck layer that represents the latent space, $\mathcal{Z}$. The encoder ($\phi: \mathcal{Y} \to \mathcal{Z}$) and decoder ($\psi: \mathcal{Z} \to \mathcal{Y}$) are the solutions to the following optimization problem:

$$\phi, \psi = \underset{\phi, \psi}{\arg\min} \sum_{i=1}^{N} ||\mathbf{y}_i - \psi(\phi(\mathbf{y}_i))||_2^2 \tag{2}$$

To train our AE, we generate a set of randomly selected design parameters ($\{\mathbf{x}_i \in \mathcal{X} | i = 1, ..., N\}$) for the structures in Fig. 1 and find the corresponding reflection responses ($\{\mathbf{y}_i \in \mathcal{Y} | i = 1, ..., N\}$) using the finite difference time domain (FDTD) technique. Using the encoder part of the AE, we can reduce the dimensionality of the reflection responses into the latent space and form the feasible regions covered by each class of structures.

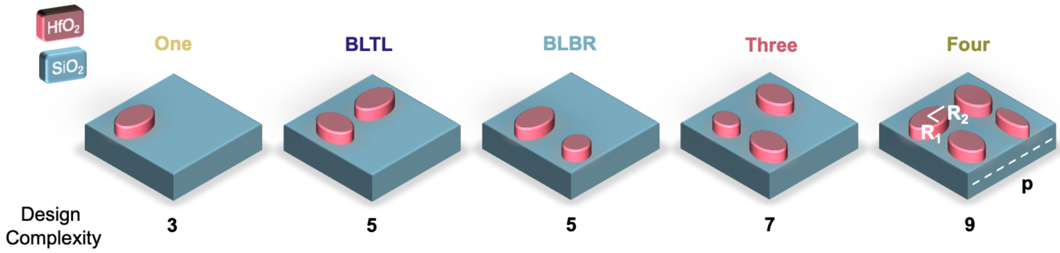

Figure 1: Schematic of the nanostructures with different complexity levels (i.e., number of design parameters) composed of unit cells with a layer of SiO_2 and ellipsoid nano antennas of HfO_2. The design parameters are periodicity of the unit cells ($p \in [500, 900]$ nm) and radius of the ellipsoids ($R_i \in [60, 200]$ nm). The number of design parameters (i.e., design complexity) are shown below each structure.

To model the distribution of the manifold of the feasible response for each structure in Fig. 1, we use GMM. We consider the probability density function (pdf) of each structure as $f_Z(\mathbf{z}) = \sum_{i=1}^{N} \alpha_i g_i(\mathbf{z})$, where $\sum_{i=1}^{N} \alpha_i = 1$ and the g_i are Gaussian distributions with different means and covariance matrices ($g_i(\mathbf{z}) = \mathcal{N}(\mathbf{z}; \mu_i, \mathbf{\Sigma}_i)$). We used expectation maximization [33] method to estimate the parameters $\theta = (\alpha_1, ..., \alpha_N, \mu_1, ..., \mu_N, \mathbf{\Sigma}_1, ..., \mathbf{\Sigma}_N)$, given a series of observations $\mathbf{z}_1, \mathbf{z}_2, ..., \mathbf{z}_M$. The goal in this optimization problem is to find a θ maximizing the log-likelihood $l(\theta; \mathbf{z_1}, ..., \mathbf{z_M}) = \sum_{i=1}^{M} \log(\sum_{j=1}^{N} \alpha_j \mathcal{N}(\mathbf{z_i}; \mu_\mathbf{j}, \mathbf{\Sigma_j}))$.

After reducing the dimensionality of the response space of the training data and modeling the manifold of the feasible set of responses for each structure in the latent space using GMMs, we use Algorithm 1 for evolutionary design of nanostructures. First we reduce the dimensionality of the desired response using a trained AE. Second, we find the log-likelihood of being inside the feasible set of each class of structures in Fig. 1. We select the structures with log-likelihood larger than a threshold as the candidates of the solution to our inverse problem. Finally, for each design candidate we use a trained NN to search over the design space for the solution (i.e., structure that has a similar reflection response to the desired response). We use MSE as our loss function to predict the responses for any given set of design parameters.

3 Results

To train our model, we generate a random set of design parameters for structures in Fig. 1 and find their corresponding reflection spectra. We sample the period of the unitcells (p) between 500 nm and 900 nm and the radius of HfO_2 ellipsoids between 60 nm and 200 nm, with the fixed thickness of 350 nm in order to support reflection mode operation and satisfy the fabrication constraints. We excite the structures with normal incident light polarized in x-direction and conduct full-wave electromagnetic simulations with commercial Lumerical FDTD software to find the reflection responses of the structure in the wavelength of interest from 300 nm to 850 nm. These structures can potentially exhibit Fano-type resonances as discussed in [30].

We trained an AE to reduce the dimensionality of the response space from 550 to 2. Based on the manifold of the responses in Fig. 2, the *Four* scenario exhibits the most variate range of spectral responses in the latent space due to the dipole resonances in x-direction (co-polarized) and strong coupling of these resonances in y-direction (cross-polarized). It is also clear from Fig. 2 that *Three*

Algorithm 1: Evolutionary Design Algorithm

Result: Optimum Design with Minimal Complexity
Step 1: Map the desired response into the latent space using the trained AE
Step 2: Find the log-likelihood of the feasibility of the response for each design complexity and select design candidates with higher log-likelihoods
Step 3: Use feed forward DNN to search over the design space of the candidates and find the optimal solution

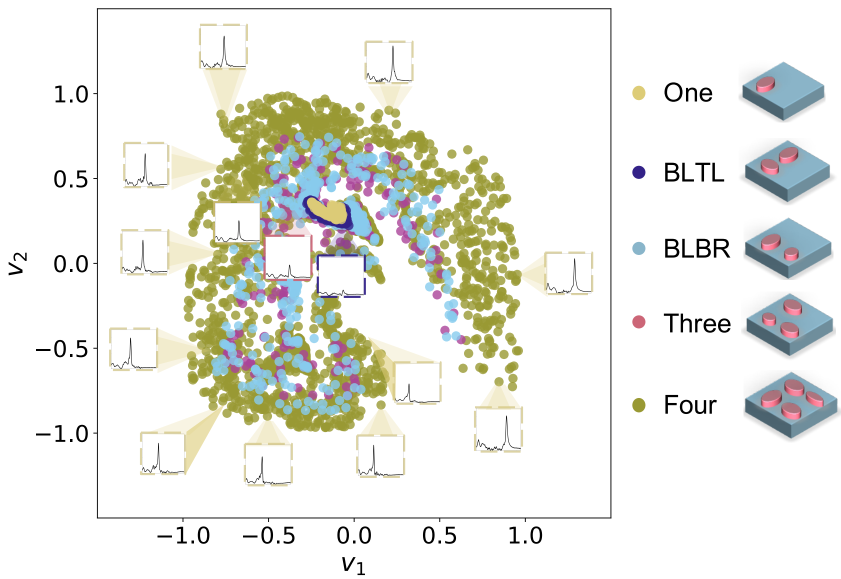

Figure 2: Representation of the responses in the latent space for the structures shown in Fig. 1. The *Four* structure, which has the highest complexity, has largest feasible region while the *One* has smallest feasible region. The changes in the responses corresponding to the movement in the latent space is shown as inset.

scenario has a substantially smaller feasible region in comparison with the *Four* scenario due to reduction in the co-polarized resonance and cross-polarized coupling. The *BLBR* scenario resembles the *Three* scenario since the co-polarized resonance is much stronger than single ellipsoid along the co-polarized direction which results in a similar feasible range of responses as the *Three* scenario. This is also supported by the feasible region of *BLTL* which is much smaller than *BLBR* as the *BLTL* resonances are too weak to be coupled and reach the variety of *BLBR*. The *One* scenario exhibits the smallest convex hull with lowest resonance and coupling amongst all the scenarios as expected. In addition to the range of feasibility, the latent space representation provides insightful information about the classes of responses of in different structures. As Fig. 2 shows, the resonances shift to left as we move counter-clockwise around the edge of the responses of the *Four* structure. Also moving from the outside of the feasible set toward the center results in significant reduction in the amplitude of the resonances. This shows that adding more ellipsoid nanoantennas results in expansion of the manifold of responses in a wide range of frequencies, and peaks with higher quality factors become achievable.

The results for two inverse designs are shown in Fig. 3(a) and (b) with the corresponding optimal design parameters, normalized mean squared error (NMSE), and log-likelihood for each structure in Table 1 and Table 2, respectively. The spectrum in Fig. 3(a) corresponds to a Gaussian spectrum with 620 nm as the centering wavelength. It can be concluded from the results that the *Four* ellipsoids

Table 1: Design parameters (in nm), NMSE, and log-likelihood for responses in Fig. 3(a). T, B, L, and R refer to Top, Bottom, Left, and Right, respectively. R_1 is the radius along x-axis and R_2 is the radius along y-axis for each ellipsoid.

	Design Parameters										
Structure	p	R1BL	R2BL	R1BR	R2BR	R1TL	R2TL	R1TR	R2TR	NMSE	$\log(p)$
One	897	179	64	0	0	0	0	0	0	0.892	-656.51
BLTL	546	79	79	0	0	153	132	0	0	0.876	-457.69
BLBR	809	153	143	163	121	0	0	0	0	0.459	-4.14
Three	780	168	144	168	144	145	98	0	0	0.397	-4.06
Four	833	823	160	823	160	823	160	160	121	**0.238**	-0.97

Table 2: Design parameters (in nm), NMSE, and log-likelihood for responses in Fig. 3(b). T, B, L, and R refer to Top, Bottom, Left, and Right, respectively. R_1 is the radius along x-axis and R_2 is the radius along y-axis for each ellipsoid.

	Design Parameters										
Structure	p	R1BL	R2BL	R1BR	R2BR	R1TL	R2TL	R1TR	R2TR	NMSE	$\log(p)$
One	683	64	64	0	0	0	0	0	0	0.892	-434.96
BLTL	882	787	111	0	0	174	89	0	0	0.880	-133.34
BLBR	736	132	121	132	132	0	0	0	0	**0.378**	-5.59
Three	700	168	121	168	98	121	98	0	0	0.411	-8.00
Four	700	823	823	823	160	121	121	160	121	0.416	-2.69

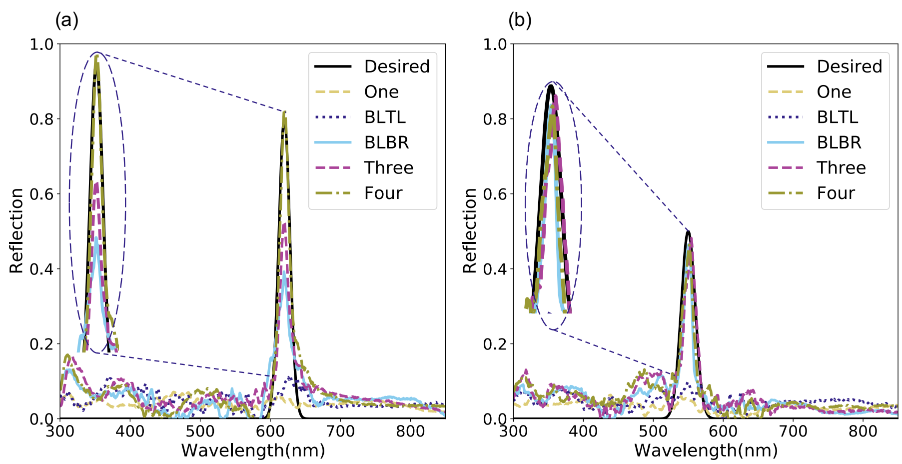

Figure 3: Results for two desired responses and optimized responses achieved by the structures in Fig. 1 using the evolutionary design algorithm. (a) A Gaussian shape reflection response with mean at 620 nm and sigma 6 nm and (b) a Gaussian with mean at 550 nm and sigma 10 nm. The corresponding design parameters, NMSE, and log-likelihood are in Table 1 and Table 2, respectvely

structure results in a lower NMSE while *BLTL* and the *One* cannot produce a response similar to the desired spectra. For the desired response shown in Fig. 3(b), however, the *Three* and *BLBR* structures result in a better design and lower NMSE in comparison to the *Four* which shows that the simpler structure would be a better option. This supports our claim regarding the ability of the evolutionary-based method for solving the inverse design with minimal design complexity. The response in Fig. 3(b) resembles a weaker cross-polarized coupling of dipole resonances compared to the desired response in Fig. 2 (b). This supports the lower NMSE of the predicted responses by *BLBR* and the *Three* for the desired response in Fig. 3(b). However due to the lack of strong co-polarized and cross-polarized couplings in *BLTL* and the *One* scenarios, the selected desired responses are not feasible with these two structures.

4 Conclusion

In this paper, we demonstrated that the proposed evolutionary design approach could significantly facilitate the inverse design of nanophotonic structures and provides the optimal solution while evolving toward the least complex structure. By providing multiple solutions (using feasibility score provided by GMM) with different degrees of freedom, our model guides the user to select the best structure with the simplest design complexity. By applying the technique to a dielectric metastructure design problem, we achieved the optimum nanostructure for a certain desired response while minimizing the geometrical complexity. Lastly, this can be extended to a wide range of design problems- fluid mechanics, material science, and electronics, to name a few.

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