Global Inverse Design across Multiple Photonic Structure Classes Using Generative Deep Learning

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Understanding how nano- or micro-scale structures and material properties can be optimally configured to attain specific functionalities remains a fundamental challenge. Photonic metasurfaces, for instance, can be spectrally tuned through material choice and structural geometry to achieve unique optical responses. However, existing numerical design methods require prior identification of specific material–structure combinations, or device classes, as the starting point for optimization. As such, a unified solution that simultaneously optimizes across materials and geometries has yet to be realized. To overcome these challenges, a global deep learning-based inverse design framework is presented, where a conditional deep convolutional generative adversarial network is trained on colored images encoded with a range of material and structural parameters, including refractive index, plasma frequency, and geometric design. It is demonstrated that, in response to target absorption spectra, the network can identify an effective metasurface in terms of its class, materials properties, and overall shape. Furthermore, the model can arrive at multiple design variants with distinct materials and structures that present nearly identical absorption spectra. The proposed framework is thus an important step towards global photonics and materials design strategies that can identify combinations of device categories, material properties, and geometric parameters which algorithmically deliver a sought functionality.

1. Introduction

A central challenge in contemporary materials and photonics research is understanding how intrinsic material properties can be optimally combined with nano- or micro-scale structuring to deliver a target functionality. Metasurfaces, for instance, hold the potential to become a vital component for many next-generation optical technologies due to their ability to manipulate the propagation of light within an ultracompact footprint.[1] More broadly, by leveraging subwavelength nanostructures and the intrinsic dispersion of constituent materials, tailored changes in the amplitude and phase of incident wavefronts can be precisely engineered, along with desired spectral characteristics. This new level of control has enabled and accelerated critical developments in fields such as flat optics,[1–3] quantum communications,[4] and holography.[5,6] However, our ability to meet increasing demands in the performance of metasurfaces, and photonic structures in general, faces roadblocks due to the complexity of the materials and structural design spaces that are currently accessible.

From the perspective of a researcher or practitioner in the field, enabling a desired set of optical characteristics today typically involves a prior understanding of the capabilities of different categories of devices or nanostructures. For instance, ultra-strong field confinement may lead one to start with a plasmonic architecture, while high transmission applications would lead one to ensure the use of materials that present low extinction coefficients in the wavelength range of operation. Designing photonic structures that meet application-specific objectives thus entails identifying the ideal intersection of material properties, structural composition, and fabrication process (or device class), as specific combinations are more likely to yield desired functional characteristics. It is only once a device or photonic structure category has been identified that numerical optimization methods typically enter the picture to optimize and refine performance characteristics.

Conventional optimization methods, which rely on numerical simulations that solve Maxwell’s equations, have shown remarkable capabilities in designing nanophotonic structures and are now commonly used.[7] However, they can be computationally costly and are often intractable for large-scale designs or high-dimensional design spaces.[8,9] As a result, data-driven approaches based on machine learning (ML) have been extensively explored in order to tackle challenging photonics design problems.[10,11] Current state-of-the-art machine learning methods involve training neural networks to learn the
underlying relationships between photonic structures and corresponding optical phenomena. A trained neural network can, in principle, instantaneously generate designs with substantially lower computational costs than optimization-based methods. A wide range of neural network and machine learning architectures have been investigated for the design and characterization of materials.\textsuperscript{[12–15]} In the photonics context, 1D tandem networks were used to design core-shell nanoparticles,\textsuperscript{[16]} multilayer thin films,\textsuperscript{[17]} and supercell-class metasurfaces.\textsuperscript{[18]} However, such network architectures are only applicable to simple photonic structures for which geometric and material properties can be described by a vector of discrete parameters.\textsuperscript{[19]} In contrast, photonic devices with complex freeform geometries cannot be well-represented by discrete variables, but offer the potential to achieve new functionalities and greater device performance.\textsuperscript{[20]}

For these structures, image-based generative networks have successfully designed various types of metasurfaces, including ones with silver\textsuperscript{[21]} gold,\textsuperscript{[22]} or silicon\textsuperscript{[23]} meta-atoms and other topological features. Further studies have combined image-based ML with optimization algorithms to yield even greater model performance.\textsuperscript{[24,25]}

Despite the significant progress in image-based photonics design, existing studies are limited to designing the two-dimensional structural topology (or geometry) for a single class of metasurface or nanophotonic structure. In addition, the material properties and out-of-plane parameters (e.g., layer thicknesses) of the explored structures are typically held constant. The central limitation identified earlier remains: prior knowledge of which category of structures or devices may deliver a specific functionality is needed before initiating the optimization procedure (whether machine learning-based or otherwise). However, human intuition on the optimal nanostructure category — the initial conditions for a numerical optimization procedure — can often go awry when faced with competing design goals. Thus, a unified “global” materials and photonics inverse design approach that can define both the materials and structure (beyond 2D) across multiple classes of photonic structures has yet to be demonstrated, but could fundamentally change how we approach the design and optimization of photonic structures and metamaterials. Moreover, such a capability could prove critical to the design of nonlinear and phase-changing platforms where optical response depends heavily on material composition and fabrication process.\textsuperscript{[26]}

In this study, we present an image-based deep learning framework for the inverse design of photonic structures across multiple materials and device categories. Our approach combines the advantages of material property and structural parameter prediction, enabled by 1D tandem networks, with the freeform design capabilities of image-based deep learning. This is accomplished through a versatile image-encoding technique where material and structural parameters such as refractive indices, plasma frequencies, layer thicknesses, resonator geometries, and metasurface classes are embedded within the discrete “RGB” channels of colored images. Although we show multiparametric encoding through different shades of color in a 3D array (as an initial demonstration), we note that this information can also be encoded via higher-dimensional matrices or data structures that extend beyond the “RGB” color system. The encoded images are used to train a customized conditional deep convolutional generative adversarial network (cDCGAN), which we evaluate by inputting a variety of target absorption spectra. In response to the input spectra, the network generates corresponding metasurface designs that are validated through full-wave electromagnetic (EM) simulations. To determine network accuracy, performance, and generalizability, the simulated spectra are compared to the input targets. Through this process, we demonstrate that the network simultaneously optimizes the material properties and 2.5D structuring across multiple classes of metasurfaces, thus validating the feasibility of a global inverse design framework that accounts for all the parameters which govern the optical behavior of photonic structures. We note that “global” in this context refers to the network’s ability to perform a global search within the surveyed design space.\textsuperscript{[8,26]} which includes material properties and freeform topology, but the network does not guarantee that the final generated device is globally optimal.

2. Results and Discussion

We consider two classes of absorbing metasurfaces in developing and demonstrating our inverse design approach (Figure 1a). First, we consider metal-insulator-metal (MIM) structures, where a thin dielectric layer is sandwiched between two metal layers (one uniformly deposited and the other lithographically patterned). This class of metasurface exhibits a relatively broad Lorentzian-shaped absorption response supported by each individual resonator, which renders this type of structure highly-amenable to thermal emission and energy harvesting applications.\textsuperscript{[27,28]} Next, we consider hybrid dielectric metasurfaces with a metal film substrate, which take advantage of a cavity effect to produce an asymmetric, narrow-band Fano resonance that is well-suited for optical sensing and detection.\textsuperscript{[29]}

As seen in Figure 1b, the first step of our encoding method involves capturing the planar geometries (G) and material properties of the metasurface resonator (M), followed by the thicknesses of the dielectric layer (T), for both MIM and hybrid dielectric metasurfaces. We then encode G, M, and T into the red, green, and blue channels of a colored image. Within our encoding scheme, the red-channel represents the plasma frequency \(M = \omega_p\) and shape of the dielectric resonator in an MIM structure. The green-channel represents the real refractive index \(M = n\) and shape of the dielectric resonator in a hybrid dielectric structure. The remaining pixels in the blue-channel are used to define the thickness of the dielectric layer (in nanometers) for both metasurface classes. Thus, a red-blue color scheme indicates MIM structures while green-blue indicates hybrid dielectric structures (red-green image combinations are undefined). With this strategy, in addition to representing resonator geometry, different colors on an image can be used to describe unique combinations of material and structural parameters, which in turn yield significantly more variation in achievable optical responses than single-material approaches.

Though the described material properties can be denoted by individual values instead of entire image channels, the presented channel-encoding method offers several key advantages.
First, it combats the well-known noise-related artifacts found in image-based ML techniques such as generative adversarial networks (GANs)\cite{8,21} by ensuring that the encoded properties are appropriately weighted towards the network’s final predictions. A detailed analysis of models trained on several property-encoded neurons versus models trained on whole image channels is found in the Supporting Information. Additionally, in principle, our approach only requires small modifications to the input dimensions of an existing model (e.g., changing from a $64 \times 64$ to $64 \times 64 \times 3$ matrix), which allows us to leverage existing model optimization and training techniques without significantly increasing training costs. Furthermore, the presented method is capable of representing spatially-varying material properties along the entire physical structure, which enables the design of 3D or complex gradient-index and metal alloy-based structures that are, in principle, amenable to existing fabrication methods.\cite{49} A demonstration of this design capability is shown in Figure S6, Supporting Information.

Our training dataset consists of 20,000 metasurface unit cell designs, represented as image-vector pairs, derived from seven shape templates: cross, square, ellipse, bow-tie, H, V, and tripole-shaped. Detailed information regarding these designs
are found in Figure S1, Supporting Information. MIM and hybrid dielectric structures are captured within 3.2 × 3.2 and 7.5 × 7.5 μm² unit cells, respectively. Each design was converted into a 64 × 64 × 3 pixel “RGB” image using the rules established above. A single pixel therefore corresponds to a minimum feature size of 50 nm (MIM) and 120 nm (hybrid dielectric), which is well-within feasible fabrication range.\[31,50\] Furthermore, we employed a Gaussian filtering post-processing procedure (described in the Supporting Information) to enhance device performance and fabricability. Finite-difference time-domain (FDTD) simulations were performed on the designs (Lumerical) to obtain an 800-point absorption spectrum vector (from 4–12 μm) for each structure. Low quality designs (defined in the Supporting Information) were removed from the training set to maximize the model’s utility and performance.\[36\] Figure S2, Supporting Information illustrates the peak absorptions and resonance wavelengths of the spectra represented in the final training dataset.

During the color-encoding step, the Drude model plasma frequencies of the metal resonators (ωp = 1.91 PHz for gold,\[31\]ωp = 2.32 PHz for silver,\[32\]and ωp = 3.57 PHz for aluminum\[33\]) were used to encode the red channel, and the real refractive indices of the dielectric resonators (n = 2.41 for zinc selenide,\[34\]n = 3.42 for silicon,\[35\]and n = 4.01 for germanium\[35\]) were used to encode the green channel. The encoded material properties are based on optical constants from the same mid-infrared wavelength range as the simulations. A range of dielectric thickness values (100–950 nm) were used for the blue channel. To support the “RGB” color scheme, all encoded values were normalized from 0 to 255.

Using the encoded images, we trained our image-based deep learning model using a GAN-based architecture. GANs have been recognized as the best-performing type of generative networks,\[39\]a class of neural networks that can directly find multiple solutions to a given problem. Other types of networks that fall in this category include variational autoencoders (VAEs)\[50\]and mixture density networks (MDNs).\[53\] Recent developments in GAN technology have led to numerous GAN-variants, including but not limited to: the Self-Attention GAN (SAGAN),\[36\]Deep Regret Analytic GAN (DRAGAN),\[37\]StyleGAN,\[38\]Wasserstein GAN (WGAN),\[39\]and the Least Squares GAN (LSGAN).\[40\] Here, as an initial proof of concept, we tested our framework using a modified cDCGAN architecture, as shown in Figure 2a. cDCGANs have previously been used to generate domain-specific images in response to input conditions.\[41–43\] Implemented in the PyTorch framework, the cDCGAN consists of a generator and a discriminator. Initially, batches of absorption spectra (y) are fed into the generator, along with a latent vector (z), to generate “fake” images (G) that are similar to the “real” images (x) from the training set. The latent vector is sampled from a random uniform distribution and allows the generator to map a probability distribution to a design space, thereby enabling a one-to-many mapping.\[28\] Both G and x are then fed into the discriminator (D), which attempts to distinguish the generated images from the real. Thus, the generator is trained to produce convincing images that deceive the discriminator, while the discriminator is trained not to be deceived—a competition which leads to the joint and stepwise improvement of both networks via their loss functions. These loss functions are calculated using the binary cross-entropy criterion, and the complete model interaction is represented as:

\[
\min_{G} \max_{D} J(G, D) = E_{x \sim P_{data}(x)} \left\{ \log D(x, y) \right\} + E_{z \sim P_{z}(z)} \left\{ \log \left(1 - D(G(z, y)) \right) \right\}
\]

where E is the expected result, \( P_{data}(x) \) is the training data distribution, \( P_{z}(z) \) is the latent vector distribution, \( \log(D(x, y)) + \log[1-D(G(z, y))] \) is the discriminator loss (\( L_{D} \)), and \( \log(D(G(z, y))) \) is the generator loss (\( L_{G} \)). During training, the objective is to maximize \( L_{D} \) and \( L_{G} \). We note that our definition of the \( L_{D} \) differs from the original GAN implementation, where \( \log[1-D(G(z, y))] \) is minimized instead, since this was shown to not provide sufficient gradients.\[53,54\] To improve the performance of the cDCGAN, we applied one-sided label smoothing and mini-batch discrimination.\[44,45\] Unlike previous cDCGAN implementations, our approach relies on adversarial training without explicitly guiding the generator towards known images,\[21\] thereby achieving a greater degree of generalization that is unconstrained by pre-existing images. Over 40 different cDCGAN architectures were trained through extensive hyperparameter tuning, and the optimized architecture can be found on Figure S3, Supporting Information. Several alternative parameter-encoding schemes were also trained and presented in Figure S4, Supporting Information, where models trained on several neurons (to represent encoded properties) were compared to models trained using the entire “RGB” channels. The validation losses of each method are reported in Tables S1 and S2, Supporting Information, and the color-encoding approach is shown to exhibit the best performance among the tested encoding schemes. After training the cDCGAN, we developed an image processing workflow to convert the generated images into full 3D metasurface designs (Figure 2b). In this workflow, the material property \( (\omega_{p} \text{ or } n) \) and thickness values \( (t) \) are calculated by taking the average pixel-values in their respective channels (based on structure classification), then reversing the normalization performed in the encoding step. Additional details regarding this process can be found in the Supporting Information.

In the GAN-metasurface design process, new materials were specified in the EM simulation software using the generated \( \omega_{p} \) or \( n \) values. We note that new materials created in this manner may not be compatible with fabrication schemes which rely on conventional materials. However, the presented material definition scheme allows the model to freely predict a continuum of material properties that are otherwise lost or disregarded due to categorical approximations, which enables a wider range of material property-driven designs. For example, metamaterials using dielectrics embedded with custom nanoparticle formulations can yield materials with effective refractive indices that can be deterministically tuned.\[46–48,50\] Prior studies have also employed nanoscale metallic alloying to achieve tailored plasma frequencies.\[57\] Highly granular material-level predictions, as we show are possible here, would therefore enable additional degrees of freedom for materials optimization, which may in turn yield novel optical responses.

We evaluated the performance of our trained cDCGAN and image processing method by inputting a set of absorption
spectra (coupled with randomly sampled latent vectors) and analyzing the resulting designs. Since the GAN may produce a distribution of designs with potentially varying degrees of accuracy,[8,51] ten different latent vectors were generated for each target spectrum, which were then used as inputs to the network. Each design is verified using numerical simulation, then the design (and corresponding latent vector) with the lowest mean-squared error to the target is reported as the final design. Figure S7, Supporting Information shows the distribution of designs (across different latent vectors) for several input targets, where we observe that each design variant has over 90% accuracy in comparison to the input target. Following this procedure, Figure 3 presents a series of tests performed with inputs that originate from the validation dataset (10% of the training dataset). Here, the blue lines represent randomly selected inputs (across both classes of structures), and the orange lines are the simulated spectra of the cDCGAN-generated designs. Images of the corresponding structures (direct outputs of the network) are shown to the right of each plot. Below each image are the associated material property (\(\omega_P\) or \(n\)) and dielectric thickness values, which are derived from the aforementioned decoding scheme. Figure S8, Supporting Information shows the equivalent results for inputs from the training dataset. We observe that in each test case, the network predicted the class of structure that corresponds with its particular type of spectral response. Specifically, when Fano-shaped spectra of various hybrid dielectric structures were passed into the network, the network exclusively generated hybrid dielectric structures (or green-blue images). Similarly, Lorentzian-shaped inputs yielded only MIM structures (or red-blue images). The generated images suggest that the network was capable of: 1) learning the distinguishing features and optical responses between the two explored classes of metasurfaces, and 2) using this information to predict the appropriate class based on the nature of the input spectra. In addition, across a wide range of input spectra, we observe that the network synthesized designs that are noticeably different from the known structures (either in resonator shape or property/thickness). Despite
this difference, the generated designs exhibit responses that strongly match the input targets. Thus, these results show that our network is not simply mimicking designs from the training dataset. To a degree, the cDCGAN is capable of learning the underlying relationships between structure, material, metasurface class, and optical response to provide new yet accurate design solutions that extend beyond the training data.

To assess our network’s ability to solve arbitrarily-defined design problems, we tested the network using “hand drawn” target spectra. These targets are derived from the Fano resonance and Lorentzian distribution functions and have no associated design or structure. We evaluated the cDCGAN’s performance across a wide range of inputs by using each function to create 200 spectra with amplitudes ranging from 0.5 to 0.9, and resonance wavelengths ranging from 5 to 9 µm, for 400 total test spectra. Figure 4a,b show several results of the Fano-shaped and Lorentzian-shaped targets, respectively, where a strong match between the targets and simulated designs can be observed. A statistical evaluation of the entire test dataset is reported in Figure 4c (for the Fano-shaped targets) and Figure 4d (for the Lorentzian-shaped targets). Here, the histograms illustrate the number of test spectra which reside in specific MSE value ranges. Dashed-red lines indicate the average mean-squared error (MSE) of the Fano-shaped and Lorentzian-shaped targets, which equal to $8.5 \times 10^{-3}$ and $2.9 \times 10^{-3}$, respectively. Through these plots, we note that the accuracy of the Fano targets is lower than the accuracy of the Lorentzian targets. However, further analysis of the training dataset (Figure S2, Supporting Information) and the individual test results (Figure S5, Supporting Information) reveal that the low-accuracy regions of the Fano-shaped structures correspond to regions that are not well-represented by the training data, whereas the high accuracy of the Lorentzian-shaped spectra can be explained by the wide spectral range of the MIM structures. Therefore, the performance of the Fano-shaped designs can potentially be improved by expanding the training data and design space.

In principle, the “one-to-many” mapping capabilities of GANs allow the deep learning model to generate multiple answers to a given problem. In the context of photonics design, this “one-to-many” feature could provide an assortment of design options from which the designer can select from. Accordingly, to harness the full potential of our property-embedded cDCGAN, we evaluate and report the network’s ability to generate multiple designs for a single target spectrum. To ensure consistency, this “diversity test” was performed on several target spectra. As seen in Figure 5a,b, we queried the cDCGAN with Fano-shaped and Lorentzian-shaped spectra, respectively. For each spectrum (shown in their individual plots), a second query was performed after resampling the latent vector and slightly perturbing the
starting spectrum. While not perturbing the spectrum still produced unique results on the second run (as shown in Figure S7, Supporting Information), adding small perturbations (<0.01 shifts in amplitude at various wavelengths) increased the overall uniqueness of the new designs. It can be observed that for each of the Fano-shaped and Lorentzian-shaped inputs, the network is able to generate two designs with distinct resonator geometry, material properties, and/or dielectric thicknesses. Importantly, though the designs have varying levels of differences, their absorption spectra remain approximately the same. The diversity of “one-to-many” structures for a target spectrum is tied to the available shapes and materials that the network was able to learn from, and allows us to make use of the non-uniqueness problem that is traditionally a limiting factor in inverse design approaches in photonics. A training dataset with a larger variety of materials and geometries could certainly yield a wider panel of designs for a given target, thereby providing end-users a range of materials and geometric designs that can deliver the same spectral response.

While the presented inverse design framework was intended to generate arbitrary material predictions as a means to enable additional degrees of freedom for geometry and materials optimization, a key limitation of the presented approach thus far is that constituent materials with arbitrarily-defined properties are generally more difficult to fabricate or synthesize than conventional materials. Accordingly, to enhance the capabilities of the proposed framework in terms of fabricability and accessibility, we demonstrate that the GAN can be used with a look-up table to substitute the predicted material properties with the closest properties derived from standard materials (shown in Figure 6). In particular, Figure 6a shows a series of tests where the input targets are Fano-shaped spectra. Here, the GAN predicted...
arbitrary geometries, thicknesses, and refractive index values of 2.48, 2.32, and 2.58 (from left to right). We observe that the simulated structures match well with the target responses (as previously demonstrated).

Next, to implement the look-up table, we substitute the GAN-generated values of $n$ with those of the closest materials found in a publicly-available database,[61] including: CdSe ($n = 2.44$), GaSe ($n = 2.38$), and CdTe ($n = 2.68$).[58–60] In Figure 6b, we perform a similar set of tests with Lorentzian-shaped spectra, where the predicted materials are substituted with Au and Ag.[31,32] In both cases, after repeating the simulations, we observe that the material approximations maintain ≈90% accuracy in comparison to the GAN’s true predictions. Thus, we demonstrate an alternative approach at using our inverse design framework to achieve designs with greater accessibility (while maintaining reasonable accuracy). We also note that some materials identified through this approach are unique and do not exist in the training dataset (CdSe, GaSe, and CdTe). However, by virtue of the GAN-based approach outputting a new material parameter (refractive index or plasma frequency) as its prediction, we are able to identify other materials (beyond the training data) that can meet the requirements of a newly sought target. We believe this highlights a notable strength of our approach, because class-based machine learning-based methods are restricted to predicting material categories that are only available in the training dataset. As we demonstrate here, our approach enables a new degree of generalization and design flexibility by allowing practitioners to access more materials than those represented by the training data. While the particular examples we presented show that the GAN predicts values which fall within the range of real materials, we acknowledge that the GAN may also predict properties beyond the current scope of conventional materials. However, we expect the accuracy of such material approximations to improve as material libraries, and material accessibility in general, continue to develop and grow.

3. Conclusions

In summary, we present a deep learning-based photonics design framework that enables the simultaneous prediction of metasurface topology, material properties, and out-of-plane structural parameters across multiple classes of metasurfaces. Our framework is centered on a conditional deep convolutional generative adversarial network (cDCGAN) and a multiparametric-encoding strategy in which the colors of an image are encoded with various material and structural properties. By accounting for the global parameters which govern the optical behavior of metasurfaces (material, structure, and device class or fabrication process), our approach overcomes the key limitations of previously-demonstrated generative models, where only a few of the aforementioned design criteria were considered. Evaluation of our model’s performance reveals that it is capable of generating not only accurate and distinct solutions...
from the training and validation datasets, but also multiple design alternatives and material recommendations for a single target by taking advantage of the “one-to-many” mapping capabilities of GANs. To account for potential fabrication or material constraints, a property-based look-up mechanism can be paired with the model’s predictions to identify readily-available materials that serve as reasonably-accurate substitutes. The presented encoding scheme is easily adaptable to existing generative models that are integrated with optimization algorithms.

Though only two classes of metasurfaces were explored in this study (metal-insulator-metal and hybrid dielectric resonators), we believe that the results here validate the feasibility of a deep learning-based global photonics design solution aimed at describing all physical aspects of a structure. Alternative encoding schemes with greater complexity, such as higher-dimensional tensors, may therefore be employed to capture more categories of photonic designs as well as more information regarding a structure’s physical properties. To achieve a more generalized inverse design framework, future studies may directly incorporate other fundamental optical properties of materials (e.g., real and imaginary refractive indices, magnetic permeability, etc.) into the model. In this regard, a multi-pole Lorentz–Drude oscillator model with multiple parameters can also provide higher-accuracy fits over alternative wavelength ranges. More broadly, the presented methodology can be adapted to a wide range of materials design problems, including mechanical metamaterials and other synthesis-driven design challenges. Thus, our proposed framework offers a path towards a global machine learning platform that can allow practitioners and researchers to identify optimal combinations of materials, geometric parameters, as well as device categories to meet complex and demanding performance goals in a range of physical systems.

Supporting Information
Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest
The authors declare no conflict of interest.

Data Availability Statement
The data that support the findings of this study are available from the corresponding author upon reasonable request.

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