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Inverse Engineering of Absorption and Scattering in Nanoparticles: A Machine Learning Approach

Inverse Engineering of Absorption and Scattering in Nanoparticles: A Machine Learning Approach

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***Abstract*—We use a region-specified machine learning approach to inverse design highly absorptive multilayer plasmonic nanoparticles. We demonstrate the design of particles with a wide range of absorption to scattering ratios (i.e., cloaked absorbers and bright absorbers) and for different visible wavelengths.**

Keywords—convolutional neural networks, scattering and absorption, nanoparticles, inverse design, machine learning.

I. Introduction

Machine learning has shown a great potential to accelerate photonic modeling and inverse design [1]. The neural network is trained to learn the underlying dynamics of the wave-matter interaction and subsequently the trained network is used to design photonic systems with the desired performance. This process is different from iterative optimization approaches and does not require continuous access to a photonic simulator.

Here, we report using convolutional neural networks (CNN) to inverse design multilayer plasmonic nanoparticles maintaining high absorption levels. Simultaneously, our model controls the relative absorption to scattering ratio ranging from small (cloaked absorbers) to large (high-scattering absorbers) ratios.

II. Electromagnetic and Machine Learning Models

The studied physical platform is a three-layer plasmonic nanoparticle. Three scaling factors are defined to describe the geometry of the particle. The spectral responses of the particle (absorption and scattering metrics) are considered as the input data for a residual one-dimensional CNN and the three scaling factors ($\alpha_{1,2,3}$) are the outputs of the network, as illustrated in Fig. 1. A schematic of the particle is shown in the inset of Fig. 2a. Layer radiuses are related to scaling factors as $\alpha_1 = r_3/700\,\text{nm}$, $\alpha_2 = r_2/r_3$, $\alpha_3 = r_1/r_2$ allowing us to work with normalized design parameters. The model is trained in Adam with mean squared error as loss function [1]. More details about the network can be found in [3]. The training dataset consists of 2310 nanoparticles with maximum diameter of 280 nm. Consequently, the spectral response of the particles is more dynamic toward shorter wavelengths (near 350 nm) and featureless toward longer wavelengths (near 700 nm). Out of the 2310 particles, we picked 1452 particles (removing those with extremely high σ_{Ratio}). The datapoints are then augmented by 25 fold by defining various regions of interest [3], [4].

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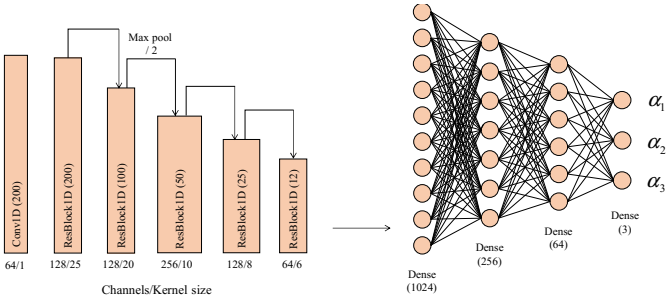

Fig. 1. The implemented CNN: The desired spectral response is the input and the three scaling factors are the outputs of the network.

We consider plane wave illumination and calculate the scattering and absorption response of the particles using the first ten Mie coefficients [5]. We are interested in particles that can efficiently absorb the incident wave (modeling a good antenna or emitter) with low (or high) scattering levels [6]. Therefore, we define two normalized metrics that are independent of the particle size, as follow,

$$\sigma_{\text{Norm}} = \frac{\sigma_{\text{abs}}}{\sigma_{\text{1, abs-max}}}, \sigma_{\text{Ratio}} = \frac{\sigma_{\text{abs}}}{\sigma_{\text{scs}}}. \quad (1)$$

Here σ_{Norm} is the ratio between the absorption cross section of the particle (σ_{abs}) and the maximum theoretically attainable dipolar absorption ($\sigma_{\text{1, abs-max}} = 3\lambda^2/8\pi$), while σ_{Ratio} is the ratio between absorption and scattering cross sections. Throughout the next section, we fix σ_{Norm} at one, pushing the particle to absorb as much as a conjugate matched dipole. By using a machine learning model, we aim to show that σ_{Ratio} can be independently controlled while maintaining high absorption, consistent with previous theoretical studies [6].

III. Results and Discussions

We assess the performance of the model through two separate test samples. For the first group of test samples, we randomly pick four sets of scaling factors (as reported in Table I), and use Mie theory to generate the scattering and absorption spectrums, σ_{Norm} , and σ_{Ratio} metrics of the corresponding particles (solid lines in Fig. 2). The generated metrics are then used as the inverse design goals and fed into the trained network as inputs. In addition, for each case we select a desired spectral

window and as such, the solid lines in Fig. 2 are limited to only specific wavelength regions. The predicted scaling factors from the network are reported in Table I. We use Mie theory once again with these predicted scaling factors and generate σ_{Norm} and σ_{Ratio} metrics, as shown by dashed lines in Fig. 2. While these metrics are plotted across the 350-700 nm range, we are only interested in the corresponding window set by the input.

TABLE I. EXACT AND PREDICTED SCALING FACTORS FOR THE DATA PRESENTED IN FIG. 2.

Panel # (Fig.2)	(a)	(b)	(c)	(d)
α_1 : exact, predicted	0.12,0.13	0.13,0.14	0.18,0.19	0.09,0.07
α_2 : exact, predicted	0.74,0.72	0.56,0.54	0.38,0.42	0.23,0.11
α_3 : exact, predicted	0.08,0.08	0.22,0.12	0.48,0.48	0.6,0.51

Inspecting Fig. 2, it can be seen that the network successfully designs particles that mimic the desired σ_{Norm} and σ_{Ratio} metrics. In addition, the retrieved values of scaling factors reported in Table I are close to the exact ones. This is an important validation step for the performance of the network, especially considering that we use a small training dataset.

For the second set of test samples we aim to design highly absorptive particles with $\sigma_{\text{Norm}} = 1$ and across two spectral windows of 350-367.5 nm and 437.5-455 nm. In each case we consider $\sigma_{\text{Ratio}} = 0.25$ and $\sigma_{\text{Ratio}} = 4.75$, corresponding to near cloaked (low-scattering) and bright (high-scattering) particles. The desired spectrum is assumed to be flat across the spectral window, however the performance may be improved by considering more realistic spectral responses [3], [4]. Relying on previous theoretical predictions [6], we expect to achieve the desired design goals (at least) across shorter wavelengths where the particle sizes allow for the excitation of higher order modes.

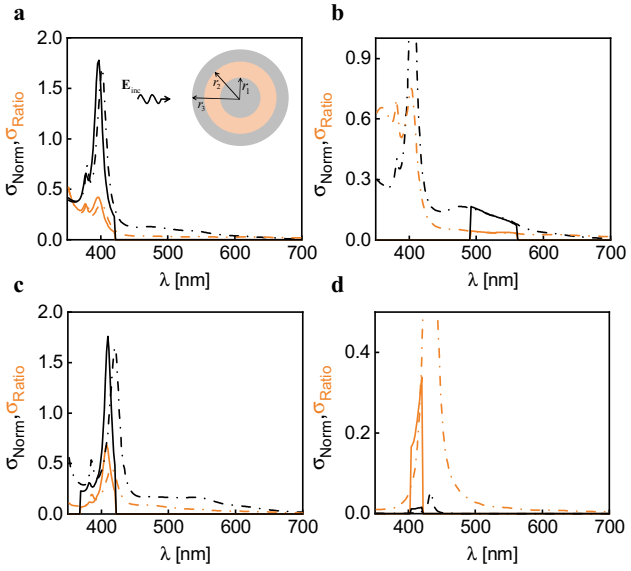

Fig. 2. σ_{Norm} (black) and σ_{Ratio} (orange) metrics calculated using Mie theory for the exact (solid lines) and predicted (dashed lines) scaling factors reported in Table I. Inset of panel (a) shows the configuration of the three-layer particle. (Core and outer shell: silicon dioxide, middle layer: silver).

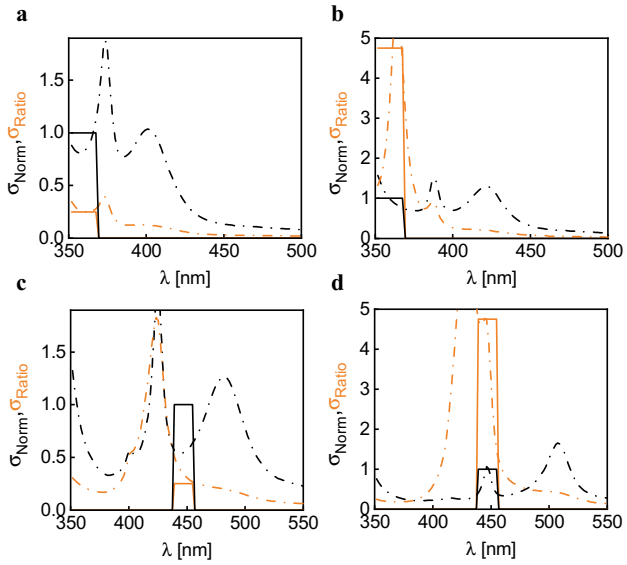

Fig. 3. Predicted σ_{Norm} (black-dashed) and σ_{Ratio} (orange-dashed) metrics to achieve $\sigma_{\text{Norm}} = 1$ and (a,c) $\sigma_{\text{Ratio}} = 0.25$, (b,d) $\sigma_{\text{Ratio}} = 4.75$ across two different spectral windows. The desired responses are shown with solid lines.

Figure 3 illustrates the performance of the network in the inverse design of such "non-physical" spectral responses. As expected, for wavelengths between 350-367.5 nm (Fig. 3a, b), the inverse designs nicely follow the desired high levels of absorption, albeit with different line shapes. The scattering levels (captured in σ_{Ratio}) also follow the desired low (panel a) and high (panel b) values. For wavelengths between 437.5-455 nm (Fig. 3c, d), the relative radiuses of the particles in the training dataset are smaller compared to operation wavelength. Consequently, the quality of the training dataset is lower, and the inverse designs only partially follow the desired goals (Fig. 3c, d). In summary, we investigated the inverse design of highly absorptive nanoparticles across different wavelength regions using a small training dataset. Our findings can find applications in design of nanoparticles, metamolecules, and antennas, where the generation of training dataset can be computationally expensive.

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