Plasmonic and dielectric nanostructures: Distinguishing size, material, and dielectric environment via machine learning

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Abstract: We employ machine learning, coupled with linear and nonlinear dimensionality reduction strategies, to distinguish between plasmonic and dielectric optical response of nanostructures and to understand the role of structural parameters and local environment.

1. Introduction

Progress in our understanding of the physics of optical materials has led to the development of novel imaging technologies at the nanoscale. While there has been much growth in the field of nanophotonics, its adoption into current technology has been hampered because of the difficulty in predicting and exquisitely tailoring the optical properties of nanostructures. Consequently, the design of a nanostructure to elicit a certain optical response remains a cyclic and difficult task. Moreover, such optimization can lead to enormous volumes of data. In recent years, dimensionality reduction and machine learning techniques have emerged as powerful computational methods for the accelerated analysis of complex datasets. Dimensionality reduction has been previously demonstrated for processing optical spectra in various fields such as astronomy [1] and medicine [2], where the goals were to speed the analysis of domain-specific properties in complex, convoluted datasets.

In this work, we explore the use of linear and nonlinear dimensionality reduction techniques for the analysis of optical properties of plasmonic and dielectric nanostructures. First, we employ linear (Principal Component Analysis) and nonlinear (t-Distributed Stochastic Neighbor Embeddings) dimensionality reduction techniques for studying optical spectra that have been analytically computed. Second, we couple this lower-dimensional study with an XGBoost-based multi-output regressor to map high-dimensional optical spectra to our 3D dimensionally reduced maps. For experimental validation, we generate spectra using a 3D full-field electromagnetic solver and evaluate these results via the presented XGBoost-based model.

2. Discussion of Methodology and Results

To demonstrate our methodology, we study optical properties of nanospheres that allows us to use an analytical function to calculate optical extinction spectra via Mie theory. To create the relevant dataset, we use the PyMieScatt [3] implementation of the Mie equations in the Python scripting language to calculate the optical spectra of nanospheres ranging from diameters of 10 *nm* to 200 *nm* with intervals of 10 *nm* that are in various dielectric environment. For the purpose of this study, we vary the dielectric values from 1.0 to 3.0 with intervals of 0.2. Materials studied include the most common (i) plasmonic materials such as Au, Ag, Cu, Al and (ii) all-dielectric materials such as Si, Ge, GaAs, GaP, and GaN (dielectric). For experimental verification, we perform finite-difference time-domain (FDTD) 3D electromagnetic simulations for nanosphere scattering calculations using the Lumerical Solutions®

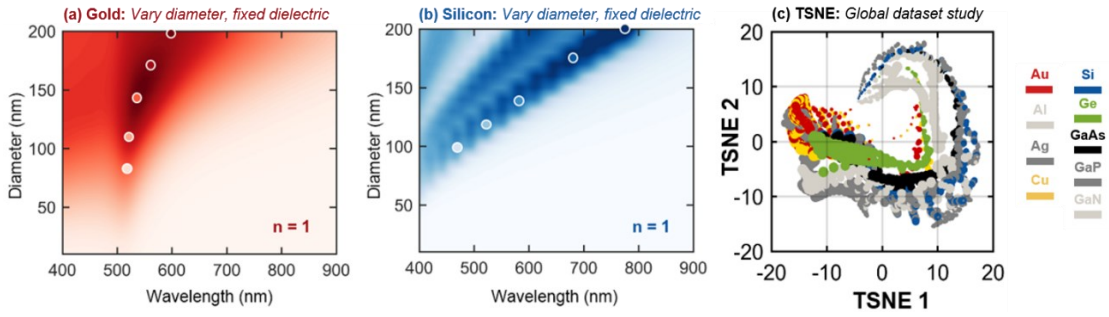

Fig 1: Two-dimensional TSNE Analysis of global dataset. Spectral maps of how (a) the plasmon resonances in Au nanospheres and (b) dielectric-Mie resonances in Si nanospheres change with respect to their diameter in air (n = 1). (c) Two-dimensional TSNE of all metallic and dielectric nanospheres as a function of diameter and environment dielectric.

solver. Specifically, we simulate the canonical plasmonic and dielectric nanospheres, that is Au and Si nanospheres. We train an XGBoost-based model to project analytically calculated optical spectra to our calculated 3D planes.

We then performed lower-dimensional studies of our analytical extinction spectra via the PCA and t-SNE technique (Fig. 1). Lower-dimensional representations are derived via extinction spectra only. We observe that the tSNE representation better separates plasmonic and dielectric materials, a characteristic not apparent in the PCA space. Furthermore, we see the similarities of Au and Cu as well as Al and Ag captured very well in both the PCA and tSNE space. We find that t-SNE exaggerates the local representation of GaN, demonstrating a key limitation of the tSNE technique.

For our experimental samples, the XGBoost model produces, on average, 1.02 times more error (RMSE) in t-SNE projections than in corresponding PCA projections when considering both plasmonic and dielectric groups. We find that Au and Si projections possess higher RMSE values than all dielectric and plasmonic groups, respectively, signifying that plasmonic and dielectric groups are being accurately separated by our machine learning model aided by the underlying dimensionality reduction scheme. Importantly, we apply this learned model to project experimentally calculated spectra to our lower-dimensional space. To better understand the contrast between various material groups, we calculate root-squared Euclidean error between corresponding nanospheres of selected groups.

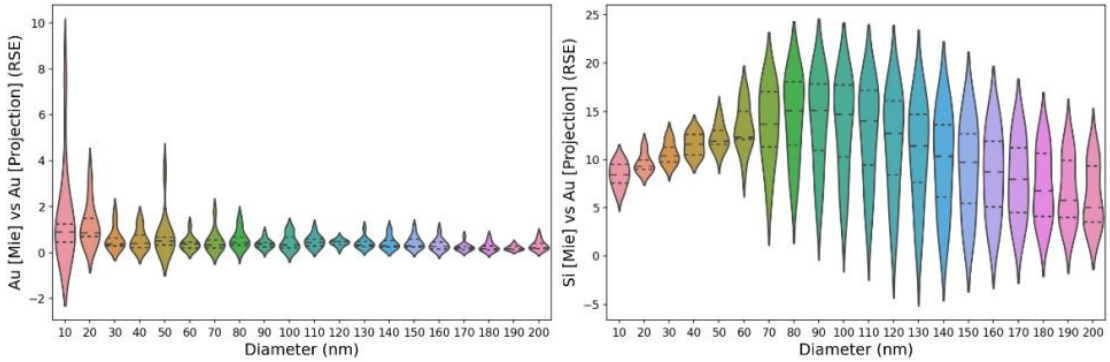

Fig 2: Root-squared error (RSE) distributions between select material groups. (a) Comparison of analytical and XGBoost-projected FDTD-calculated Au spectra. (b) Comparison of analytical Si spectra and XGBoost-projected FDTD-calculated Au spectra.

We observe high error in low-diameter projections caused by the lack of significant signal (resonance) being present in the optical response. We see a high degree of error between the Au and Si groups (Fig. 2), coinciding with trends in material dielectrics and our Fig. 1 representations. We find the lowest disagreement between the two groups at low diameters, where less resonance effects are present (Fig. 2).

3. Conclusions

We have shown that machine learning, when coupled to linear and nonlinear dimensional reduction techniques, are highly effective in providing insights about optical response of nanostructures. Dimensionality reduction techniques are capable of effectively learning lower-dimensional representations of nanospheres consistent with intrinsic physical properties. Furthermore, we find that we can separate experimentally simulated nanostructures based on intrinsic material properties using our machine learning model.

4. References and Acknowledgments

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