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Predictive residual neural networks for optical trapping of small particles

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ABSTRACT

Optical tweezers provide a non-contact method to trap, move, and manipulate micro- and nano-sized objects. Using properly designed dielectric and plasmonic nanostructure configurations, optical tweezers have been tailored to create stable and precise trapping for nanoscale objects. Recent advances in numerical optimization techniques allow further enhancement in nanoscale optical traps through inverse optimization of such configurations. One of the main challenges in such optimization approaches is the time-consuming nature of full-wave simulation of nanostructures and postprocessing steps to extract optical forces. To address this challenge, we introduce a surrogate solver based on residual neural networks that can accurately predict the forces exerted on a nanoparticle. Our results illustrate the possibility of capturing the highly nonlinear dynamics of local optical forces using moderate-sized datasets, particularly appealing to the inverse design of optical tweezers.

Keywords: Optical trapping, metasurfaces, residual neural networks, near-field engineering, predictive modeling, machine learning

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1. INTRODUCTION

Since their first demonstration in 1970 by Arthur Ashkin [1], optical tweezers have found notable applications in several scientific areas and industrial fields ranging from biology and physics to medical sciences and manufacturing [2]-[5]. Traditional optical tweezers rely on focused laser beams to create an optical trap. However, and due to the diffraction-limited laser focal spots, such an approach is not well-suited for stable and high-precision trapping of nanoscale objects. In addition, the size of the focal spot is inversely proportional to the attainable forces on the particle and the depth of the trapping potential. More recently, and to circumvent these limitations, plasmonic and dielectric nanostructures have been extensively used to create highly focused hotspots for efficient nanoparticle trapping [6]-[11]. Particularly, inverse design techniques have been employed to improve the local power in the particle's location, enabling better trapping performances and low-power operations of nano-tweezers [12]. In addition to single particle trapping, in some applications, it is desired to simultaneously trap multiple particles even with different characteristics [13]. To address this need, multiparticle trapping systems are of interest, with recent proposals using quasi-BIC systems, Fano resonances, and spin-dependent lenses [13]-[16]. Efficient design and modification of such systems to ensure robust and precise trapping of particles with various shapes, sizes, and materials creates a demand for efficient modeling and response prediction of large and multiparticle trapping systems. Clearly, an important challenge in the inverse design of optical tweezers is the time-consuming full-wave simulation step. To address this challenge, in this article, we propose a surrogate solver for vectorial forces exerted on a dielectric nanoparticle. This solver is tested on a large dielectric metasurface, emulating non-periodic wave-matter interaction over a gradient metasurface [17].

2. RESULTS AND DISCUSSION

Our platform consists of a dielectric metasurface with twenty distinct elements per unit cell size of $L = 2\lambda_0$, where λ_0 is the free-space wavelength set at 1550 nm. The metasurface consists of twenty silicon pillars with a refractive index of 3.48 and height of 300 nm with different widths, placed on a thin silicon dioxide substrate with the refractive index of 1.444

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and thickness of 100 nm. The metasurface is backed by a silver mirror with 200 nm thickness, ensuring operation in reflective mode. Figure 1a illustrates the electric field amplitude distribution around a sample metasurface illuminated with a plane wave from the top, indicating several hotspots in the vicinity of the surface. A spherical glass nanoparticle with a diameter of 40 nm is considered in the vicinity of the surface, 30 nm above the top of the silicon elements. The area above silicon elements is filled with water (refractive index of 1.3109) creating a small refractive index contrast between the particle and background medium. Our goal is to train a residual neural network to efficiently predict the optical forces (i.e., $\mathbf{F}\cdot\mathbf{x}$ and $\mathbf{F}\cdot\mathbf{y}$) exerted on the spherical particle. Note that as the metasurface elements are invariant in the z-direction, the force component in the z-direction is zero with our network trained to predict the x- and y- components of the optical force. In addition, the presented method is readily extendable to two-dimensional metasurfaces to allow for nonzero forces in the z-direction.

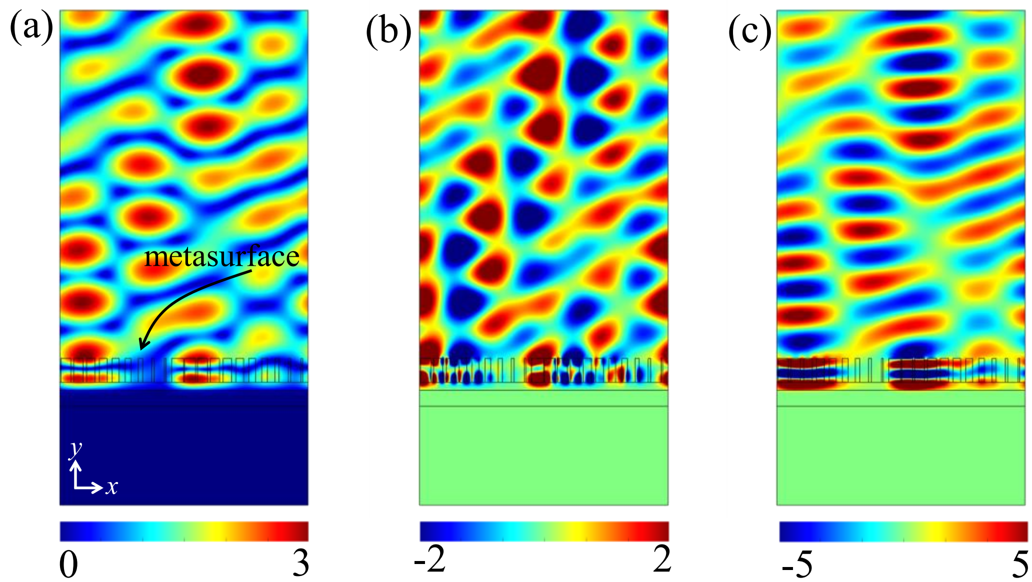

Figure 1. (a) Distribution of the electric field amplitude in the vicinity of the dielectric metasurface under study. The field is normalized to the amplitude of the incident field. The (b) x- and (c) y-components of force exerted on a glass nanoparticle with a diameter of 40 nm. Both color bar units are $\mathrm{fN}\ 10\mathrm{mW}^{-1}\mu\mathrm{m}^2$.

Data-driven approaches such as neural networks rely on high-quality datasets for the training of the model to accurately capture the complex dynamics of the system. Consequently, and depending on the platform, optical forces must be calculated through full-wave simulations for a large number of training cases. While some techniques have been explored to enhance the performance of the network with smaller training datasets [18]-[21], in general, dataset generation is the most computationally expensive portion of the design approach. Relevant examples include recent works on using data-driven approaches for predicting the scattering, resonances, and absorption of different classes of nanostructures [22]-[27]. For optical forces exerted on a small particle, it is possible to reduce this time by using some available approximate formulas, as discussed below. We note that using other approximations such as RCWA [28] can also boost the calculation efficiency and reduce the time required to generate a quality dataset. Exact forces can be calculated by integrating the Maxwell stress tensor over the closed surface of the particle [29],

$$\mathbf{F}=\oint_S \overline{\overline{T}}\cdot\mathbf{ds},\quad \overline{\overline{T}}=\varepsilon_0\left(\mathbf{EE}+c^2\mathbf{BB}-\frac{1}{2}\left(\mathbf{E}\cdot\mathbf{E}+c^2\mathbf{B}\cdot\mathbf{B}\right)\overline{\overline{I}}\right). \tag{1}$$

For a dipolar particle, the force can be approximated as $\mathbf{F}=1/2\,\mathrm{Re}[\nabla\mathbf{E}^*\cdot\mathbf{p}+\nabla\mathbf{H}^*\cdot\mathbf{m}-ck_0^4/6\pi(\mathbf{p}\times\mathbf{m}^*)]$ which can be further simplified to $\mathbf{F}=1/4\nabla\left(\mathrm{Re}\left[\alpha_{ee}\right]|\mathbf{E}|^2\right)$ for a small dielectric non-chiral particle [29]. Here α_{ee} is the electric polarizability of the nanoparticle [30]. Figure 2 illustrates the accuracy of this formula in our studies for a sample metasurface.

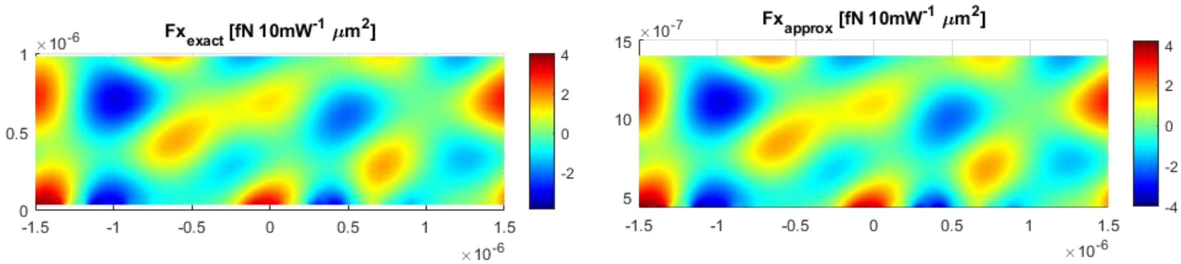

Figure 2. Approximate (right) and exact (left) value of $\mathbf{F}\cdot\mathbf{x}$ calculated using dipolar approximation and the integration of Maxwell stress tensor over the particle, respectively. In both cases, fields are calculated using COSMOL full-wave simulations. The figures correspond to the lower portion of the force distribution shown in Figure 1b.

Given the negligible difference between the exact and approximate forces in this case, we generate the training dataset using approximate forces for 601 points across the surface, 30 nm above the silicon pillars. Figures 1b and 1c show the x- and y-components of the force for a sample metasurface. We note that the performance of our model is independent of the data generation method. For larger particles and when dipolar approximation is not relevant, direct integration of the Maxwell stress tensor should be used to generate the data. Using a dataset of 25,000 metasurfaces (corresponding to less than two samples for each metasurface element), first, we downsample the force from 601 parameters to 201 parameters, taking every third parameter. Then we implemented two residual neural networks to independently predict the $\mathbf{F}\cdot\mathbf{x}$ and $\mathbf{F}\cdot\mathbf{y}$ force components. Overall, 90% of the data is used for training and 10% is used for testing and validation. In addition, and to better understand the impact of the size of the dataset on the overall performance, the first network is trained using the entire 25k datapoints, and the second network is trained with 15k datapoints. A moving average filter with a window size of 5 is then applied to the results to minimize noise. Figure 3 illustrates the results indicating accurate prediction in both cases.

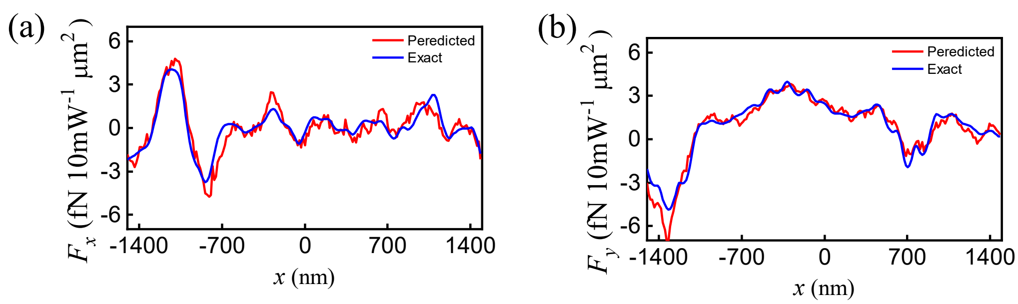

Figure 3. Exact and predicted force (a) along the x-direction and the (b) y-direction, applied to the nanoparticle 30 nm above the silicon elements. The models are trained with 25k and 15k datapoints respectively.

Finally, we also designed a single model to simultaneously predict both force components. Using the previous models as a starting point, we have achieved very accurate predictions for both components using 15k datapoints, as illustrated in Figure 4.

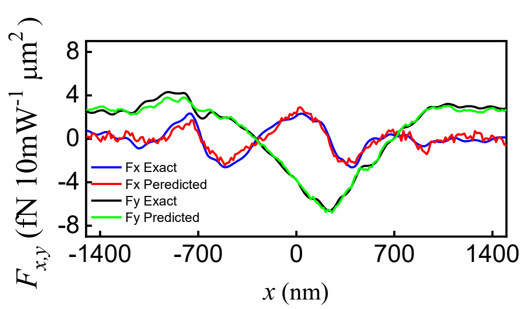

Figure 4. Exact and predicted forces applied to the nanoparticle 30 nm above the silicon elements. A single model is constructed to predict both forces, trained with 15k training datapoints.

3. CONCLUSION

We implemented a residual neural network to accurately predict the local vectorial forces exerted on a nanoscale dielectric particle in the vicinity of a complex metasurface. Given the complex and nonlinear local wave-matter interaction at the interface, our results demonstrate the potential of neural networks to operate as surrogate optical force and optical trapping potential solvers. Our results are particularly relevant to the inverse design of optical nano-tweezers. In addition, and given the high accuracy of the results for the relatively low number of training datapoints in the design space, our approach may be used to predict the response of more complex nanostructures such as topology-variant structures [31]-[35] and disordered structures [36]-[38] as well as nonlinear and quantum metasurfaces [39]-[40].

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