Exploring Multiple Network Architectures to Solve Selected Challenges in Computational Nanophotonics

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Abstract: We present our most recent contributions to explore the use of different architectures for artificial neural networks to simulate the interaction of light with nanostructured materials. Among others, we exploit graph neural networks to substitute a finite-difference time-domain scheme and Fourier neural operators as surrogate solvers for electromagnetic scattering problems. For the latter, we highlight the opportunity to solve tasks in the context of the inverse design of free-form scatterers with an optical response on demand.

Methods and techniques from the field of computer science, and especially from the field of machine learning, currently penetrate optics and photonics and are explored for selected purposes. While multiple networks were studied for designing specific nanophotonic devices [1, 2], we explore from a slightly different perspective the use of particular architectures of artificial neural networks for the more general task of solving Maxwell's equations or replacing traditional techniques to simulate the interaction of light with nanostructured photonic materials.

One example of the latter would be the finite-difference time-domain (FDTD) method, where simulations are made by discretizing Maxwell's equations in space and time on a grid and evolving an initial field through a given spatial domain using a leap-frog-scheme. In our work, we have been using graph neural networks (GNN) for the same purpose. By representing the electromagnetic field distribution as a graph, we successfully train a GNN to propagate the field for a fixed time step. Despite relatively small domain sizes in training, our GNN can extrapolate to arbitrarily large domains while preserving high prediction accuracy. Additionally, our approach works on square grids, the backbone of any FDTD, but also on arbitrary unstructured meshes. Hence, this GNN architecture opens novel opportunities to bypass a notorious shortcoming of the traditional FDTD approach.

On the other hand, we introduce a Fourier neural operator network as a surrogate solver for Maxwell's equations. The FNO is not a general-purpose Maxwell solver but requires a set of structures and their scattering response as training data. The model is trained on a diverse set of free-form electromagnetic scatterers, and we compare its performance to a state-of-the-art convolutional architecture (UNet). We show that FNO requires significantly fewer data to reach the same accuracy as UNet. Further, we show the inverse design of free-form three-dimensional optical elements using our pre-trained model. We obtain feasible devices while achieving a significant speedup over conventional means for inverse design. The model is geared to predict structures feasible for fabrication with additive manufacturing technologies. The FNO makes it possible to design structures with disparate objective functions and is, in that sense, a general-purpose tool.

References

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