Physics-informed neural network for inversely predicting effective electric permittivities of metamaterials

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Abstract

We apply a physics-informed neural network framework for inversely retrieving the effective material parameters of a two-dimensional metamaterial from its scattered field(s). We show that by employing a loss function based on the Helmholtz wave equation, we can model the performance of a metamaterial disc-shaped structure and split-ring resonator with great promise and demonstrate the dependance of resonant behavior on the homogenized electric permittivity distribution profile generated by our network.

1 Introduction

Metamaterials (or 'metasurfaces' in the planar case) are artificially engineered composites that demonstrate highly controllable manipulation of electromagnetic fields resulting in electromagnetic responses that are not achievable in naturally occurring materials. These materials comprise of building blocks with dimensions that are much smaller than the interacting wavelength(s) and can therefore, be considered as effectively homogeneous materials whose performance is dictated by the artificially structured unit cells or 'meta atoms' rather than the fundamental properties of the constituent materials, resulting in novel phenomenon such as negative refraction, cloaking effects and sub-diffraction imaging (1). In recent years, an impressive body of research has successfully established data-driven design and optimization models based on deep learning for deriving the complex, and often non-intuitive, relationships between metamaterials and their response(s), which are dictated primarily by Maxwell's equations for electromagnetics (2). A recent paradigm for tackling inverse problems in electromagnetics, typically the retrieval of structural and material properties that lead to a target response, are physics-informed neural networks (PINNs), which is an indirectly supervised learning framework for solving partial differential equations using limited sets of training data (3; 4). In this work, we describe the use of PINNs for 'homogenizing' two distinct meta atom designs , namely a disc and a split-ring resonator (SRR) by inversely predicting their effective electric permittivity distributions from simulated scattered electric field(s). Homogenization simply means the resultant electric fields are identical to those scattered by a hypothetical continuous medium with the same effective material properties, in line with well-established 'effective medium theory'(4). SRRs are essentially oscillators formed by a combination of an inductive element (the ring) and a capacitive

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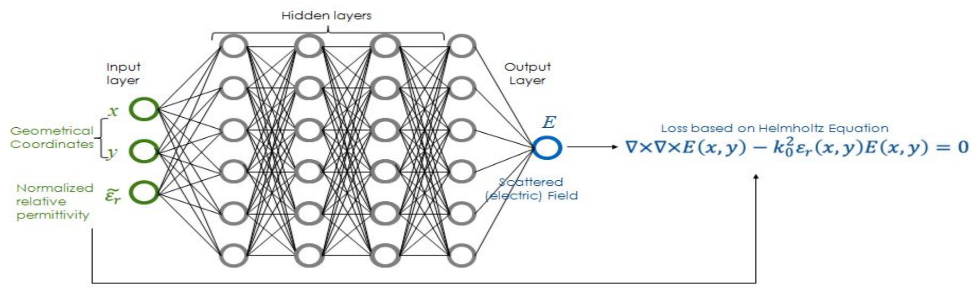

Figure 1: Representative diagram of the physics-informed neural network model with 6 layers. Each hidden layer contains 250 neurons. A physics-driven loss function based on the Helmholtz equation is used to train the model

element (a split or gap region in the ring). When the split-ring is in resonance with the frequency of the incident light, large local fields are observed in the gap region. The parameter that dictates this local field enhancement is the effective electric permittivity coefficient of these non-magnetic metamaterials. To the best of our knowledge, this work is the first demonstration of the effect of the accuracy of the PINN-based inverse model on the nature of the SRR's complex, resonant behavior.

2 Methods

We consider two distinct metamaterial unit cell structures for this study; one is a 2D silicon disc (electric permittivity = 11.9) surrounded by air (electric permittivity = 1) and the other is an aluminium SRR on a silicon substrate (electric permittivity = 11.9). Figure 2(a) and 3(a),(d) depicts their dimensional parameters. The resonance frequency of the SRR is designed to be at 0.225 GHz for an incident wavelength of 1.33m. We compute the electric field as a function of the metasurface's spatial coordinates (here, *x* and *y*) using the Helmholtz wave equation in the frequency domain for linear, non-magnetic, weakly inhomogeneous materials, which is given by equation 1:

$$\nabla \times \nabla \times E(x,y) - k_0^2\epsilon_r E(x,y) = 0 \tag{1}$$

where, *E* denotes the electric field, k_0 is the free space wave number and ϵ_r represents the relative electric permittivity distribution. We use $k_0 = 5$ for both the disc as well as the SRR.

The physics-driven, mean squared error (MSE) loss function is expressed in terms of the residue of the Helmholtz equation and is computed as:

$$MSE = \frac{1}{N}\sum_{i=1}^{N} |F(x_i, y_i)|^2 \tag{2}$$

where,

$$F(x_i, y_i) = \frac{\partial^2 E(x,y)}{\partial x^2} + \frac{\partial^2 E(x,y)}{\partial y^2} + k_0^2\epsilon_r E(x,y) \tag{3}$$

Equation 2 is used to train the DNN and optimizes the architecture to generate an effective permittivity spatial profile that results in an electric field (*E*-field) that is identical to that of the original metasurface design. We use a simple, fully connected feed-forward neural network, as shown in figure 1, with an input layer comprising of three neurons, namely, *x*,*y*, and normalized relative permittivity $\tilde{\epsilon_r}$ defined as:

$$\tilde{\epsilon_r} = \frac{\epsilon_r - \epsilon_{min}}{\epsilon_{max} - \epsilon_{min}} \tag{4}$$

This is followed by 4 hidden layers of 250 neurons each and an output layer with a single neuron for the predicted *E*-field distribution *E(x,y)*. The input-output relationship of the network is denoted by *E(x,y,θ)* as a surrogate for the PDE solution to the Helmholtz equation, wherein θ is a vector containing the trainable weights and biases of the network. We shifted and scaled the intermediate layers linearly to [-1, 1] to prevent the network from overfitting. We used the tf.gradient function in Tensorflow 2.4.1 to calculate the partial derivative terms in equation 3. We used the $\sigma_s = sin(\pi.s)$

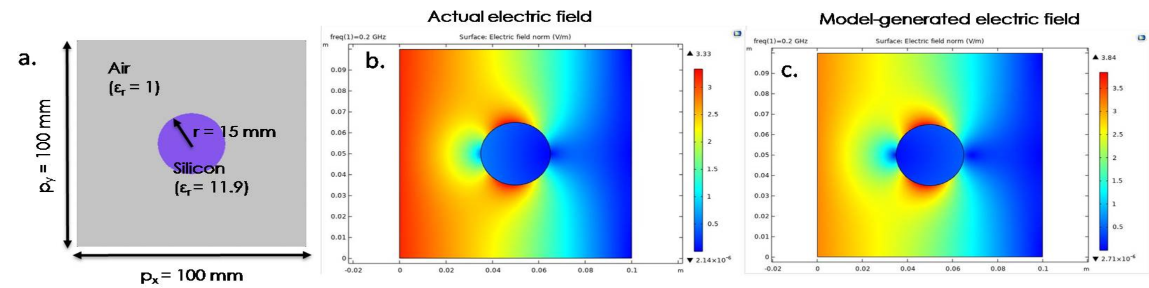

Figure 2: (a) Schematic of the disc-shaped metasurface unit cell. (b) Ground truth electric field. (c) The electric field calculated by our model.

activation function, which was found to be most suitable for our chosen wavenumber $(k_0 = 5)$. We chose the Glorot optimization function for initializing the weights and biases and set the learning rate to 10^{-4}. We used the Adam optimizer to update the weights and biases to reduce the MSE. For both the disc as well as the SRR geometry, the model was run for 10,000 iterations; the input data (spatial coordinates and $\hat{\epsilon_r}$) for the disc was 26,000 and for the SRR was 36,000. . We evaluated the output E-fields from our model by performing a full-wave simulation using a commercially available finite element method solver(COMSOL Multiphysics 5.6) on an Intel Core i7-9750H CPU, 2.6 GHz, 16 GB RAM.

3 Results and discussion

Figure 2(c) and 3(f) depicts the E-fields predicted for the disc and the SRR respectively. We observe that the calculated EM response, which is based on the predicted ϵ_r, agrees well with the ground truth for the disc. However, for the significantly more complex SRR, we observed a discrepancy between the predicted and the actual E-field, which we attribute to the shift in the resonance frequency for the predicted permittivities. Figures 3(b) and 3(e) show that the resonance frequency for the predicted structure blue shifts to 0.79GHz from the designed resonance at 0.225GHz.

Prior reports indicate that the accuracy of the model increases as we increase the number of training iterations (5; 6). As we were limited by the computational resources available to us, for this work, we could attempt a maximum of 10000 iterations only. The MSE achieved by optimizing the physics-driven loss for the disc was 57 and for the SRR was 276. The larger error for the SRR case can be explained by the highly sensitive dependence of the resonance phenomenon on the material properties (ϵ_r in this case).

4 Conclusion

We have used the PINN framework for retrieving the effective permittivity distributions of a simple disc-shaped meta atom as well as a complex, circular split-ring resonant geometry. Our feed forward neural network's loss function is formulated using the Helmholtz wave equation (derived from Maxwell's equations), which governs electromagnetic wave propagation in any medium. We compare the E-field generated by our network (based on the predicted permittivity distribution) to the ground truth data generated using a commercial EM solver wherein the electric permittivity values are discretely defined. We observe that for relatively simple structures such as the disc, 10000 training iterations are sufficient for demonstrating spectral performance but for a split-ring geometry, where the resonant behavior depends sensitively on material properties, the model should ideally be run for higher number of training iterations to accurately capture the spatial profile of its material properties. We envisage that these studies will help in understanding how PINN parameters should be chosen to accurately capture the responses of complex metamaterial geometries.

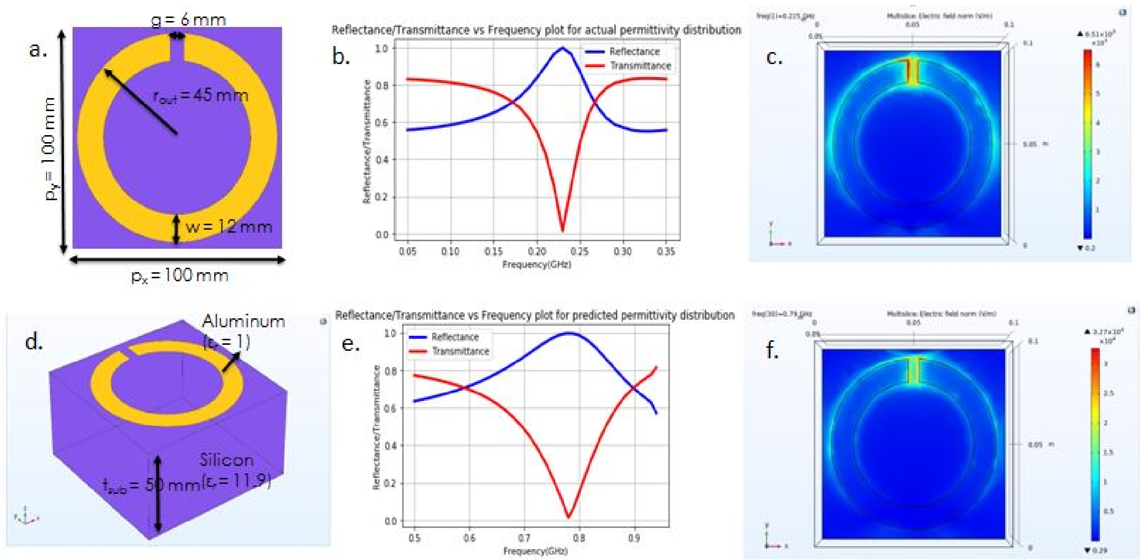

Figure 3: (a) 2D Schematic of the split-ring resonator metasurface unit cell. (b) Reflectance-transmittance plots showing the resonance for the ground truth structure (c) Ground truth electric field. (d) 3D Schematic of the split-ring resonator metasurface unit cell (e) Reflectance-transmittance plots showing the resonance for the predicted structure (f) Electric field calculated by our model

5 Broad impact

The development of simplified, data-driven design methods that avoid tedious, computationally intensive calculations, will contribute significantly towards increasing the penetration of metamaterials into applications that impact our daily lives, either as end-user devices or an integral components in high-tech assemblies. A primary outcome of the PINN framework is the simplification of the network training process via a reduction in the number of curated training datasets unlike conventional machine learning approaches. In our PINN-based approach, we do not require E-field data to converge to a solution but rely solely on the physics-driven loss to depict a metamaterial's spectral response. Here, we have essentially 'hand-tuned' our model to give us the best result, given the constraints on the computational resources available to us. The future scope of this work will prominently feature an automated selection of optimal network parameters for more complex metamaterial topologies and configurations.

References

[1] Smith, D. R., Pendry, J. B., and Wiltshire, M. C (2004) Metamaterials and negative refractive index, *Science, 305(5685):788–792.*

[2] Yao, K., Unni, R., and Zheng, Y. (2019) Intelligent nanophotonics: merging photonics and artificial intelligence at the nanoscale. *Nanophotonics, 8(3):339–366.*

[3] Fang, Z., and Zhan, J. (2019) Deep physical informed neural networks for metamaterial design, *IEEE Access, 8:24506-24513.*

[4] Chen, Y., Lu, L., Karniadakis, G.E., Dal Negro, L. (2020) Physics-informed neural networks for inverse problems in nano-optics and metamaterials, *Optics Express, 28:11618-11633.*

[5] Raissi, M., and Karniadakis, G.E. (2018) Hidden physics models: Machine learning of nonlinear partial differential equations, *J. Comput. Phys., 357: 125-141.*

[6] Raissi, M., Perdikaris, P., and Karniadakis, G.E. (2019) Phsyics-informed neural networks: A deep learning framework for solving forward and inverse problems involving partial differential equations, *J. Comput. Phys., 378: 686-707.*

Checklist

(a) For all authors...
  i. Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? **[TODO]**Yes
  ii. Did you describe the limitations of your work? **[TODO]**Yes. See Section 3 (Results and Discussion)
  iii. Did you discuss any potential negative societal impacts of your work? **[TODO]**N/A
  iv. Have you read the ethics review guidelines and ensured that your paper conforms to them? **[TODO]**Yes

(b) If you are including theoretical results...
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  ii. Did you include complete proofs of all theoretical results? **[TODO]**N/A

(c) If you ran experiments...
  i. Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? **[TODO]**No. The code and the data are proprietary.
  ii. Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? **[TODO]**Yes. See Section 2 (Methods)
  iii. Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? **[TODO]**N/A
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