‘MetaNETs’ - Accelerated discovery and design of photonic metamaterials using deep learning

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Abstract

We propose an approach based on neural networks for approximating the electromagnetic (EM) responses of mesoscale, split-ring resonator photonic metamaterials. We demonstrate that by treating the EM spectral data as time-varying sequences and the inverse problem as a single-input, multi-output model, we force our architecture to learn the geometry of the designs from the training data as opposed to abstract features thereby addressing both the forward and the inverse design problems with great promise.

1 Introduction

Optical metamaterials (MMs) are artificially structured composites that demonstrate customizable electromagnetic (EM) properties that stem from morphological feature dimensions of the order of the interrogating wavelength. MM devices are composed of periodic 2D or 3D arrays of sub-wavelength conducting elements and exhibit light-matter interactions that enable the manipulation of the effective electrical permittivity and effective magnetic permeability, therefore opening up new paths for versatile, photonic devices [3]. Traditionally, the MM design process relies heavily on the knowledge and intuitive reasoning of the researcher as achieving a target spectral behavior involves iteratively tweaking the design till the outcome is satisfactory. Starting with an initial geometry, standard numerical techniques such as the finite-difference time domain method, boundary element method are employed for solving the Maxwell’s equations for obtaining the spectral response [6]. Of late, commercially available EM solver software packages have been widely adopted by the MM community for designing metamaterials but there too, the optimization of target design depends largely on intuition.

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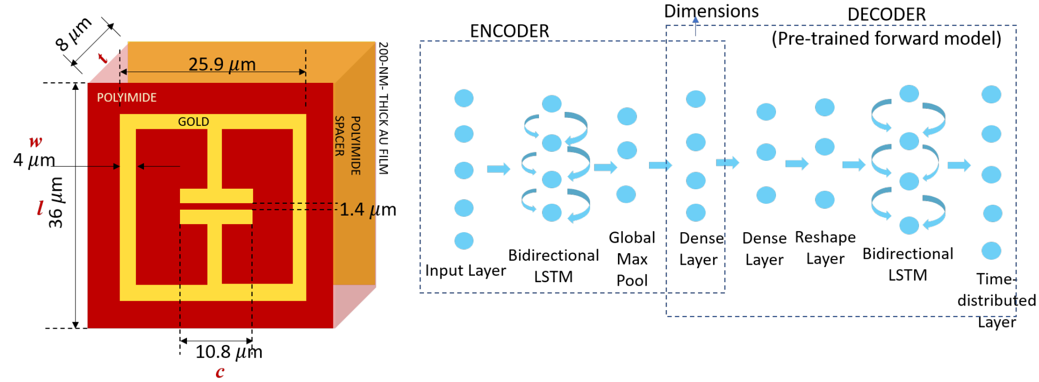

Figure 1: Annotated schematic of our chosen split-ring resonator metamaterial (left) and the MetaNETs architecture comprising of an inverse design network connected to a forward modeling network (right)

An efficient MM design scheme encompasses two aspects: the forward problem (predicting the EM response for a given geometry) as well as the inverse problem (generating the structural parameters for a desired EM response). In this work, we explore the unique property of RNNs [2] to leverage the sequential information inherent in the spectral responses. The workflow of our MetaNETs architecture is divided into two; first, the training of a forward model with the geometry as input and the corresponding spectrum as output, and second, posing the training approach for the inverse problem as a single-input, multi-output (SIMO) model using a tandem network of an encoder and a decoder with sequential input data (spectral information in this case). The dimensions and the spectra are outputs of the trained inverse model. The combined loss was controlled by fixing the weights and biases of decoder with the pre-trained forward MLP-LSTM network (dimensions-sequence).

2 Preparation of the design-EM response dataset

We consider a MM device based on split-ring resonators (SRRs) that has been designed for near-unity absorption (97%) at 1.6 terahertz (THz) [4]. Split-ring resonators (SRRs) are a MM design element type that demonstrates negative permeability and supports inductive-capacitive (LC) resonances [7] Figure 1 depicts a schematic of the device along with its dimensions. We begin by building the dataset comprising of 5169 geometries and their spectral response (calculated by solving for Maxwell's equations using first principles) using the numerical simulation package COMSOL 5.3. The geometries were generated by performing parametric sweeps over its defining geometrical parameters namely, the linewidth of the gold features (w), the thickness of the dielectric substrate (t), the length of the gold layer (l) and the width of the capacitor (split-region) (c). The corresponding absorption curves were plotted between 0.8 THz to 2.4 THz and discretized into 161 data points. The dataset was split into three parts, namely, the training set, the validation set and the test set in the ratio 70:15:15 respectively.

3 Results and Methods

3.1 The forward model for split-ring resonator-based metamaterials

The forward model is a combination of a multilayer perceptron (MLP) and a bidirectional long short-term memory (LSTM) layer wherein the inputs comprise of 16 expanded dimensions obtained by combining the four geometrical parameters (l, t, w, c) using ratios and products. We treat the 161-dimensional output as timesteps for the sequential input to the bidirectional LSTM layer and the output is then obtained through a time-distributed wrapper on the final feed-forward layer with a linear activation function. As multiple geometries can yield near-identical EM responses, L2 regularization was done for all layers to make a more generalized and robust model which can discriminate between

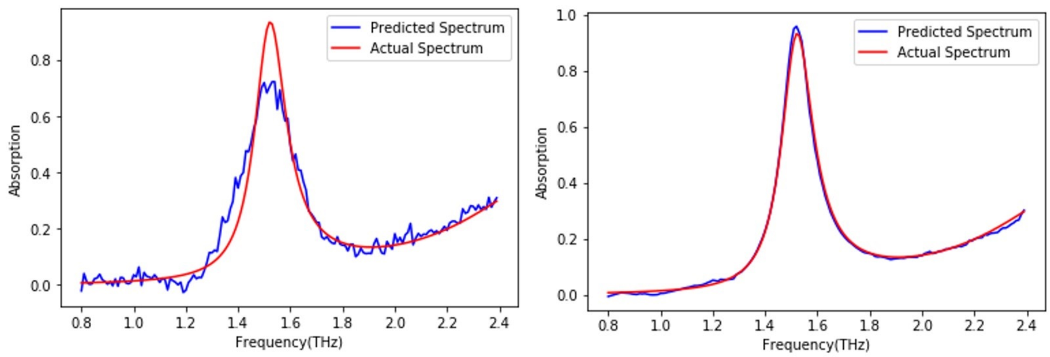

Figure 2: Performance comparison of a DNN-only (left) and an LSTM-based (right) forward model on randomly selected samples from test set

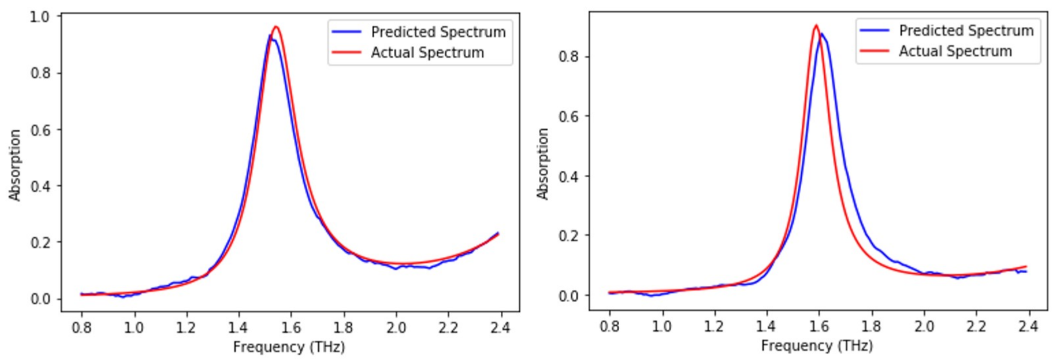

Figure 3: Comparison of predicted and actual spectra from our tandem model on randomly selected samples from test set

geometries having near identical spectra. The regularization parameter and the learning rate was set at 0.00001 and 0.0001 respectively. The architecture is trained for 1000 epochs and the mean squared error (MSE) was selected as the loss function. The training took approximately 13 hours on a standard Intel® Core™ i5 CPU @1.60 GHz with 8 GB of RAM.

In order to validate our hypothesis, that of treating the spectral response as sequence of absorption values, we compare our model's predictions to a baseline architecture without an LSTM and using a feed forward non-recurrent neural network. Figure 2 clearly depicts the superiority of the LSTM-based forward network in predicting the spectral response. Therefore, for the inverse model as well, the LSTM layer is a fitting choice considering the sequential nature of the input spectral data.

3.2 Solving the inverse problem using an encoder-decoder tandem network

Once successfully trained, the forward model was connected to an inverse model to form a tandem neural network consisting of an encoder and a decoder, wherein the decoder has the weights saved from the pre-trained forward model. The encoder input is the sequence of 161 absorption values, which are encoded to the geometry's dimensions using a combination of the LSTM layer and a MLP encompassing the architecture for the inverse predictions. Within the encoder, the MLP transforms the LSTM output features averaged over the timesteps into the dimensions (geometry). The decoder, then takes these dimensions and outputs the spectral response using the pre-trained network weights. During training, the tandem network, learns to yield the dimensional information for the SRR structures while trying to reproduce the spectral input given. The loss function is selected as MSE for both the outputs and trained for 1000 epochs. Our training approach for the tandem network is similar to autoencoder architectures used for dimensionality reduction [5] and learning latent representations

Table 1: Model evaluation (Average losses over 5 runs)

Model	Train	Validation	Test
Forward model	0.0056	0.0057	0.0056
Inverse model (spectrum)	0.004	0.0039	0.004
Inverse model (dimensions)	48.64	59.79	53.38

Table 2: Predicted vs actual values of design parameters of the SRR. All values are in micrometers. D1 and D2 are randomly selected geometries from the test set

	D1				D2			
	l	***w***	***t***	***c***	***l***	***w***	***t***	***c***
Ground truth	23.95	4.96	9.43	10.52	27.49	5.50	8.31	10.69
Predicted	23.90	4.75	9.00	11.50	27.90	5.25	8.10	10.60

[1] of data in an unsupervised manner. However, here, we force the network to learn the geometry of the MM device rather than abstract features, thus solving the inverse problem with great promise.

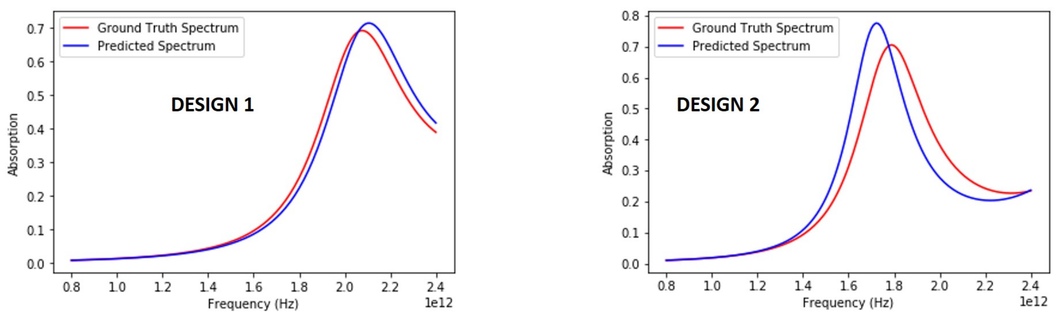

Figure 4: Comparison of EM response obtained by first principles simulation of couple of randomly selected geometries (Design 1 (D1) and Design 2 (D2)) from the test set vs target/desired EM response

Table 1 summarizes the average losses obtained for the forward and the tandem inverse models over 5 runs. In order to evaluate the capability of the tandem model to retain information about the input spectra, we randomly selected a few geometries and compared the ground truth spectra to to their corresponding spectra as predicted, from the test set. As seen in Figure 3, the predictions from our tandem model closely follows the actual curves, thereby validating our approach. As a performance test for the inverse model, we again did a random selection of a few predicted SRR geometries, computed their EM response using the full-wave EM solver, and compared them to the test set spectra from the inverse model (Figure 4). The results (Table 2) show that the SIMO approach is able to converge on a design solution without significant deviations.

4 Conclusion

In summary, our results clearly demonstrate that this method can be easily implemented for forward and inverse predictions for fairly complex geometries such as SRRs. The MetaNETs architecture developed by treating the EM response data as a time-varying sequence and using an LSTM, performs well via a robust mapping of the spectra to the geometry without much optimization. We hypothesize that architectures comprising solely of networks of fully connected multi-layer perceptrons with the frequency-dependent absorption values as features, may be learning some dependency (order) between the layers. However, when trained are unable to efficiently leverage the sequential nature of the data in the manner RNNs can, owing to their superior architecture. Additionally, we check the precision of our model's predictions by comparing with ground truth data which we generate via 'virtual' experiments wherein we solve Maxwell's equations and compute the SRR's performance using first principles. The comparison results validate our architecture as an efficient and accurate model for the design and discovery of complex metamaterials. As a qualitative indicator of computational efficiency, the COMSOL full-wave simulations for a single design took around 7 minutes on a standard Intel® Core™ i5-8250U CPU @ 1.60 GHz with 8 GB of RAM; whereas our forward model took 0.001 seconds to predict the corresponding spectra.

Broader Impact

MM devices such as the broadband absorber considered by us, have vast scope for a multitude of applications across domains as diverse as high-speed communications, photovoltaics, novel healthcare devices, stealth applications for defense amongst others, however, their technology penetration has been limited so far due to complex design processes that require advanced skills and knowledge base(s). The advent of data-driven models makes it possible to generate designs based on user-defined, on-demand device performances within fractional time durations.

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