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# Utilizing machine learning techniques for predictive modelling of absorptivity in l-shaped metamaterials

Md Adil[1,a*], Pratik Punj[2,b]

[1]Department of Mechanical Engineering, Jadavpur University, Kolkata, India

[2]Department of Mining Machinery Engineering, IIT (ISM) Dhanbad, Dhanbad, India

[a]adil.alam45@gmail.com, [b]pratik10singh@gmail.com

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**Abstract.** Metamaterials are artificially engineered materials that have properties not found in naturally occurring materials. They are designed to have specific electromagnetic or other physical properties, such as negative refraction, superconductivity or high absorptivity. They are often composed of structures on a scale much smaller than the wavelength of the phenomena they are intended to manipulate. Metamaterials have a wide range of potential applications, including in antennas, cloaking devices, and super resolution imaging. In this paper we have simulated and validated an L shaped meta material to make a data set of its absorptivity by varying different input parameters and then used these data to predict the absorptivity of any L shaped metamaterial using machine learning and it gave satisfactory results.

## Introduction

Metamaterials, artificially engineered substances that possess uncommon electrical and magnetic characteristics, have become the focus of much interest due to their potential uses in fields such as negative refraction [1-2], superlensing [3,4], and optical cloaking [5,6].

The idea behind metamaterials, where properties are obtained by controlling the boundary conditions or the phase and shape of its components, can be traced back to early explorations in the fields of acoustics and vibrations, such as Newton's research on sound transmission through air and Riley's examination of alternate structures. In recent times, Acoustic Metamaterials (AMs) have become a subject of growing interest among the scientific community, due to advancements in the measurement of sound waves and the control of feedback vibrations [7].

Metamaterials have found significant industrial applications, particularly in the field of antenna engineering, where their ability to control electromagnetic waves has led to the creation of smaller and more efficient antennas for various applications such as mobile communication, satellite communication, and radar. The use of metamaterials in antenna design has also led to the development of antennas with improved bandwidth, gain and radiation patterns, resulting in more efficient communication systems. Additionally, metamaterials have been utilized in the field of imaging and sensing, leading to the development of sensors with enhanced resolution and sensitivity. These sensors are used in applications such as medical imaging, remote sensing and security imaging, allowing for early detection and diagnosis of diseases, and remote monitoring of environmental conditions.

Metamaterial other‘s industrial applications, includes waveguiding, energy harvesting, as well as in public safety, sensor identification, high-frequency battlefield communications, improved ultrasonic sensors, solar energy management for high-gain antennas and remote aerospace applications [8-10]. Moreover, researchers from the army and air force employ metamaterials for detecting explosives, biological materials, and contamination [11-12]. The capability of metamaterials to manipulate sound wavelengths, which are much larger than light, has led navy

researchers to investigate their potential use in hiding submarines in military operations. In addition, metamaterials have found applications in civilian domains, such as the creation of sound chambers. Army engineers also utilize metamaterials to manufacture small and high-speed photonic equipment, as light is becoming increasingly important in the development of future circuit boards [13].

Metamaterials have the ability to create a "perfect" absorber with close to full absorption, a concept first introduced by Landy et al. [14]. By incorporating intrinsic loss and carefully designing the structure of the metamaterial, various types of perfect metamaterial absorbers can be created for specific wavelengths, including the microwave range , optical wavelengths [14], and infrared [15]. These absorbers enhance sensitivity in chemical and biological sensing applications [16].

There are two main approaches to creating metamaterials: forward design and inverse design [17-18]. The forward design method involves obtaining material responses through theoretical analysis, simulations, and experiments . However, this method can become expensive as the design complexity increases, as it requires repeatedly modifying material parameters and recalculating responses. In contrast, inverse design [19] has gained popularity as it involves constructing appropriate structures through optimization algorithms in a large parameter space.

The progress in Artificial Intelligence (AI) has made the concept of inverse design a practical reality. AI includes optimization algorithms like simulated annealing, genetic algorithms, particle swarming optimization, and topology optimization, which are well- established and widely employed for generating inverse designs as per the specific needs. These algorithms typically depend on intermediate results obtained through an iterative forward design process. Despite this, performing inverse design under multiple constraints remains a challenge due to the restrictions of a purely random search.

The field of artificial intelligence (AI) has seen significant advancements in recent years, with machine learning (ML) becoming a prevalent approach. The origins of ML can be traced back to the 1940s and 1950s, with the introduction of the artificial neural network and the concept of variable connection strength between neurons. However, it wasn't until the 1980s that ML truly began to gain traction, with the development of the back-propagation algorithm for training neural networks. Deep learning, a branch of machine learning, has been widely used to predict the properties of materials and design (nano)photonic devices. Researchers have used deep neural networks (DNN) to approximate the electromagnetic response of a given structure, a process known as forward prediction. For example, Peurifoy et al. trained a neural network to predict the scattering of light by multilayer nanoparticles [20]. However, when it comes to inverse design of photonic devices, which involves finding the structure that corresponds to a specific electromagnetic response, DNNs often face challenges due to the one-to-many mapping problem.

The application of machine learning (ML) in the fields of electromagnetic and light waves has led researchers to explore the use of ML in the design of other materials that manipulate, providing a powerful tool for characterizing artificial material properties and structuring materials.

Therefore, it's not surprising that Machine Learning (ML) methods have gained increasing attention for analyzing the transmission and dispersion characteristics of periodic acoustic metamaterials, which are characterized by the presence of local resonators. Reviews on the application of ML in acoustics can be found in studies such as those by Bianco et al. [21] and Michalopoulou et al. [22]. Using ML techniques, novel functional applications have been proposed, such as the optimal design of tunable mechanical filters and directional waveguides, as seen in the works of Bacigalupo et al. [23] and Gurbuz et al. [24]. In this research paper, we will explore the possibility of predicting the absorptivity of metamaterial on any particular wavelength based on its parameter for which a simulation model has been created and validated to create the dataset. The results are promising absorptivity estimation performance.

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**NARX Neural Network**

The NARX, or Nonlinear Autoregressive model with Exogenous inputs, is a type of artificial neural network that mirrors the structure of the biological neural system. It comprises interconnected nodes, each of which receives one or multiple inputs and processes them by summing them up and then passing the result through a nonlinear activation function. These nodes perform like artificial neurons. NARX networks are distinct from other types of artificial neural networks because they facilitate information flow in both directions. This allows for connections between neurons within the same layer and between current and previous layers, resulting in faster optimization of connection weights and needing fewer layers to be calibrated. As a result, NARX is a highly effective model.

Governing equation for basic NARX NN model:

$$z(m+1) = f[z(m), \dots, z(m-d_z+1);\ v(m), v(m-1), v(m-d_v+1)]$$

Or can be written as,

$$z(m+1) = f[Z(m); V(m)]$$

Here, z(m) and v(m) represent the output and input of a model, respectively. The terms $d$z and $d$v indicate the output and input memory orders, respectively, with $d$z > 1 and $d$v > 1. The vectors $T$(m) and V(m) represent the input and output regressors, respectively.

NARX (Nonlinear Autoregressive with exogenous inputs) is a highly capable type of dynamic model that has been shown to have computational capabilities equivalent to those of a Turing machine.

**Training Algorithm**

*Levenberg–Marquardt (LM):*

The Levenberg-Marquardt (LM) algorithm is a well-known method utilized for forecasting time series through artificial neural networks (ANNs). This method incorporates the benefits of both the Gauss-Newton and steepest descent methods to optimize a non-linear function that represents the sum of squares of the error. The objective of the LM algorithm is to identify the lowest possible value of this function, thus enhancing the prediction's accuracy.

$$F(t) = \frac{1}{2}\sum_{i}^{m} [f_i(t)]^2$$

*Scaled Conjugate Gradient (SCG):*

The Scaled Conjugate Gradient (SCG) algorithm is frequently utilized in the training of feedforward neural networks. It is a general optimization method that has been modified to enhance the determination of step size and direction of search. It is based on a second-order approximation as represented by an equation.

$$E(a+b) \approx E(a) + E'(a)^T + \frac{1}{2} v^T E''(a) b$$

The objective of the algorithm is to determine the optimal distance in each iteration through line search, with the goal of finding the most suitable distance to move in the search direction using equation.

$$a_{k+1} = a + l_k * p_k$$

After that, it performs the next search direction which is conjugate to the previous search instructions.

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*Bayesian regularization(BR):*

Bayesian regularization is a method employed in artificial neural networks (ANNs) for adjusting the values of weights and biases through the use of Levenberg-Marquardt optimization. The goal is to find the best combination of these values by first reducing the square error and weight, and then incorporating the weights into the objective function of the training procedure, as represented by an equation.

$$F(\omega) = \alpha\varepsilon\omega + \beta\varepsilon D$$

The Bayesian method is then employed to optimize the values of the objective parameters $\alpha$ and $\beta$.

$$P(\alpha, \beta|E, N) = \frac{P(E|\alpha, \beta, N)P(\alpha, \beta|N)}{P(E|N)}$$

**Dataset**

The illustration of the unit cell for the proposed single L-shaped metamaterial absorber, which was simulated and validated to gather data for training the neural network, is displayed in Fig. 1. Unit cell of the proposd single L shaped metamaterial absorber which we have used to gather data for neural network can be seen in Fig. 1. Proposed metamaterial has been simulated on COMSOL Mutiphysics and has been validated wih the experimental data[25]. In the suggested metamaterial, gold has been used as a material for the L shaped patch and also for the bottom metal layer. Drude model has been used to model the dielectric behaviour of the gold with theplasma and collision frequency of 16 x 10^1.2 rad/s and 13 x 10^10.5 rad/s respectively[44]. SiC has been used as the dielectric spacer with dielectric constant and loss tangent of 10.8 and 0.003 respectively. Thickness of gold and SiC has been taken as 0.27 μm(td) and0.1μm(tm)m(td) and 0.1 μm(td) and 0.1μm(tm) m(tm) respectively.

Absorption capability has been calculated using the relation A = 1 - |S11|^2 , where |S11|^2 represent the square of the magnitude of reflection coefficient.

The absorption capability of the proposed single L-shaped metamaterial absorber is determined by the amount of reflection it experiences, which is calculated by taking the difference of 1 and the square of the magnitude of the reflection coefficient, represented as |S11|^2. The absorption can be represented mathematically as A = 1 - |S11|^2.

The absorption spectrum of the single L-shaped metamaterial absorber, as measured experimentally, is presented in Fig. 2. The graph also displays a comparison between the theoretical calculations and experimental results for the case of transverse electric incidence. The theoretical calculations were made by using the dispersive model of silicon carbide's dielectric constant. As seen in Fig. 2, the simulation was able to accurately capture the presence of two strong peaks and their corresponding wavelengths.

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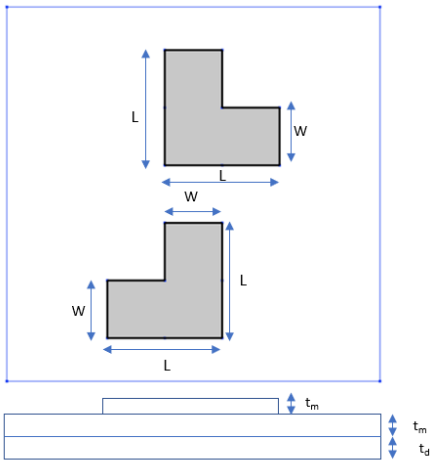


*Fig.1 Schematics of L-Shaped metamaterial*

Now two genarated data set, dielectrci constatnt, loss tangent and wavelength has been choosen as an input parameter to predict the absorptivity of the designed metamaterial. In total we have generated 1000 data points using Comsole Multiphysics.

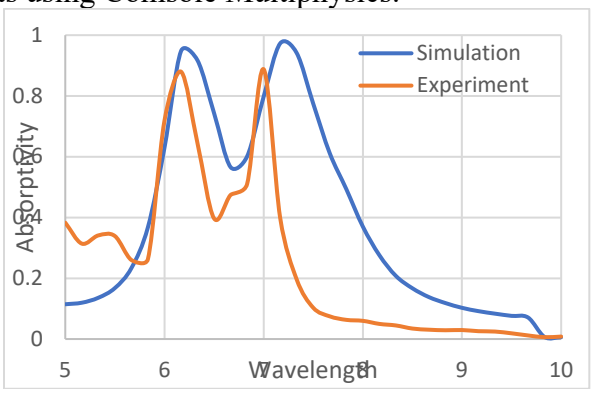


*Fig . 2 Comparision of Simulated and Experimental results*

**Performance Parameter**

In this paper, following matrices are employed to evaluate the precision of each model and to compare the performance of various training algorithm.

Mean Square Error (MSE):

$$MSE = \frac{1}{n}\sum_{t=1}^{n}(error)^2$$

Root Mean Square Error (RMSE):

$$RMSE = \sqrt{\frac{1}{n}\sum_{t=1}^{n}(error)^2}$$

Where,

$$error = actual\ value - estimated\ value$$

**Results and Discussion**

FEA analysis has been done with the following parameters using Comsole Multiphysics simulation software as shown in TABLE 1.

As can be seen in Fig. 3, with increase in dielectric constant value, wavelength for maximum absorptivivty and that for all other local maxima start to shift toward a longer wavelength.

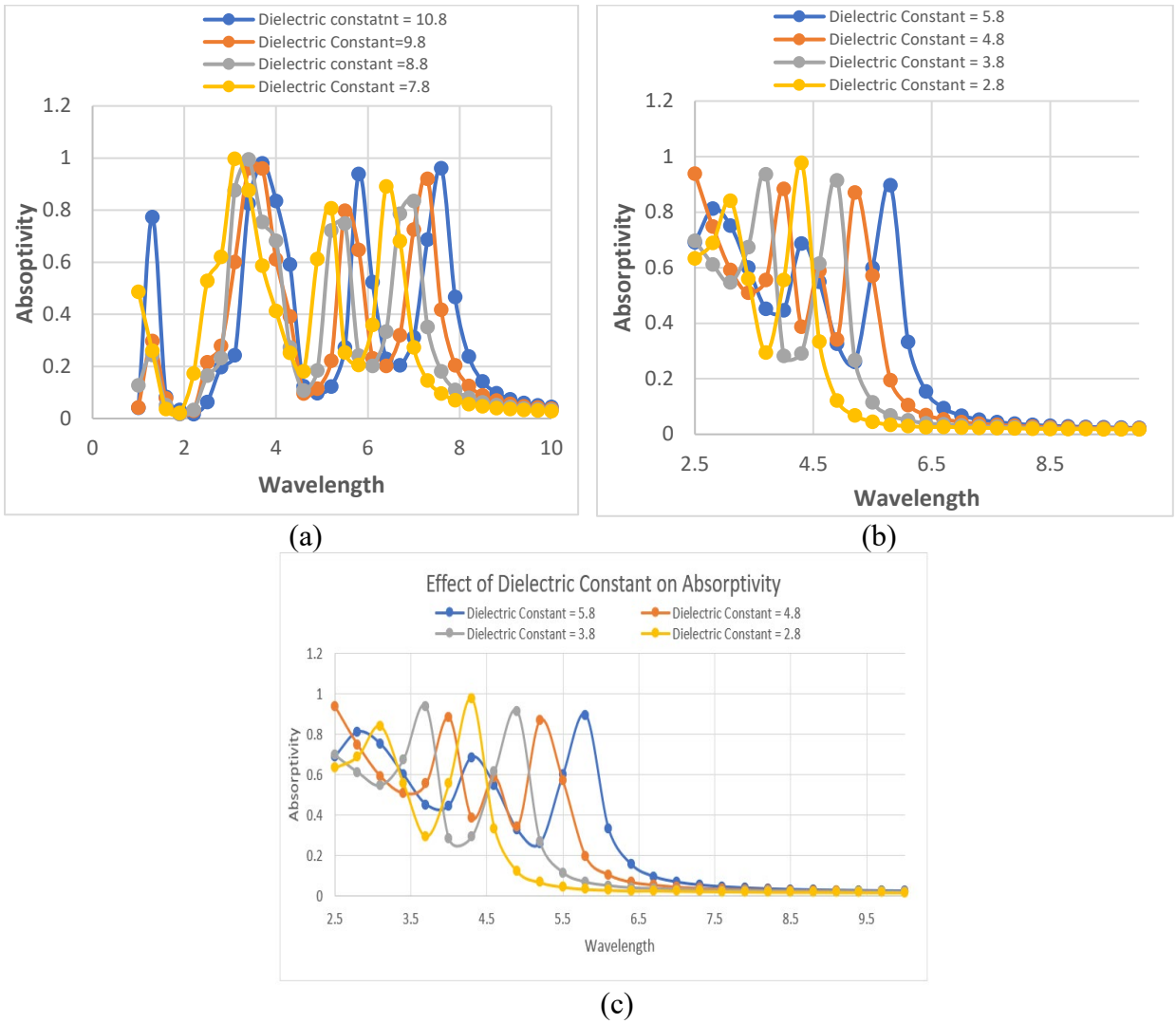


*Fig. 3 : Effect of dielectric constant on absorptivity at loss tamgent (a) 0.001 (b) 0.002 (c) 0.003*

When changing the loss tangent value for a given dielectric cpnstant we haven‘t found any change in either of the maximum absorptivity or the corresponding wavelength as can be seen in Fig. 4.

The proposed NARX NN used data collected from multiple simulations for training, testing, and validation. Whole data set has been divided in two sets (1:3) the larger set (Set 1)has further been divided in 70:15:15 ratio in random manner to train, test and validate the network while the input parameter from smaller set (Set 2) has been used to predict the value and then the result of both has been compared. The network was first trained using the Levenberg-Marquardt, Scaled Conjugate Gradient, and Bayesian Regularization algorithms, then tested, and finally used to predict the absorptivity for any arbitary input of dielectric constant, loss tangent and wavelength.

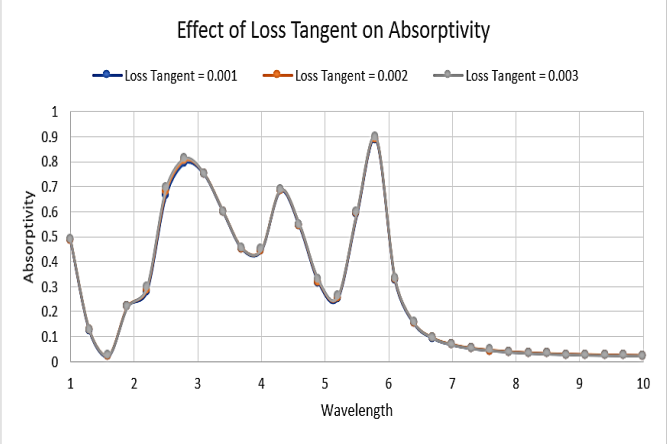


*Fig. 4 : Effect of loss tamgent on absorptivity at dielectric constant value of 5.8*

The proposed NARX NN used data collected from multiple simulations for training, testing, and validation. Whole data set has been divided in two sets (1:3) the larger set (Set 1)has further been divided in 70:15:15 ratio in random manner to train, test and validate the network while the input parameter from smaller set (Set 2) has been used to predict the value and then the result of both has been compared. The network was first trained using the Levenberg-Marquardt, Scaled Conjugate Gradient, and Bayesian Regularization algorithms, then tested, and finally used to predict the absorptivity for any arbitary input of dielectric constant, loss tangent and wavelength.

The network has been trained using the mean squared error (MSE) as the criteria, in which the network calculated the gradient and updated the weights to reach a point of minimum error.To validate the network performance, autocorrelation was used as a metric and was observed to be influenced by the value of delays. Thus, the delays were chosen in a way to ensure that the values remained within a confidence level. the autocorrelation remained within the 95% confidence level all the three algorithm. Correlation between input and errors, has also been found to be within the confidence limit at all lags, indicating that the model had captured all the features of the system and that the input and output were modeled accurately.

*TABLE.1 Performance parameter for different training algorithm on set 1*

| **ALGORITHM** | **TRAINING** | **VALIDATION** | **TESTING** |
|---|---|---|---|
| *Bayesian regularization* | 0.92644 | 0.86774 | 0.91776 |
| *Levenberg-Marquardt* | 0.89644 | 0.86196 | 0.81638 |
| *Scaled Conjugate Gradient* | 0.86635 | 0.85201 | 0.81736 |

As can be seen in the Table. 1 that *Bayesian regularization* was mos accurate while testing the network on Set 1 while other two i.e *Levenberg-Marquardt* and *Scaled Conjugate Gradient* performed almost similarly. On Set 2 *Scaled Conjugate Gradient* performed much better than the other two algorithms as can be seen in Table. 2.

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*TABLE.2 Performance parameter for different training algorithm on set 2*

| **ALGORITHM** | **RMSE** | **MSE** |
|---|---|---|
| *Bayesian regularization* | 0.46673 | 0.21784 |
| *Levenberg-Marquardt* | 0.40905 | 0.16732 |
| *Scaled Conjugate Gradient* | 0.27871 | 0.07768 |

NARX NN has been able to capture the peaks and valleys pretty accurately but the corresponding wavelength is little offset. SCG training algorithm has fared comparitively better as compared to other two when predicting the absorptivity for wavelength above 8 µm. BR algorithm resulted in most noisy response in predicting absorptivity above 8 µm wavelength while at the same time it has also predicted the absorptivity most accurately for wavelength value of upto 6µm. SCG algorithm has also been able to capture the upper and lower limit of the absortivity value as compared to other two training algorithms.

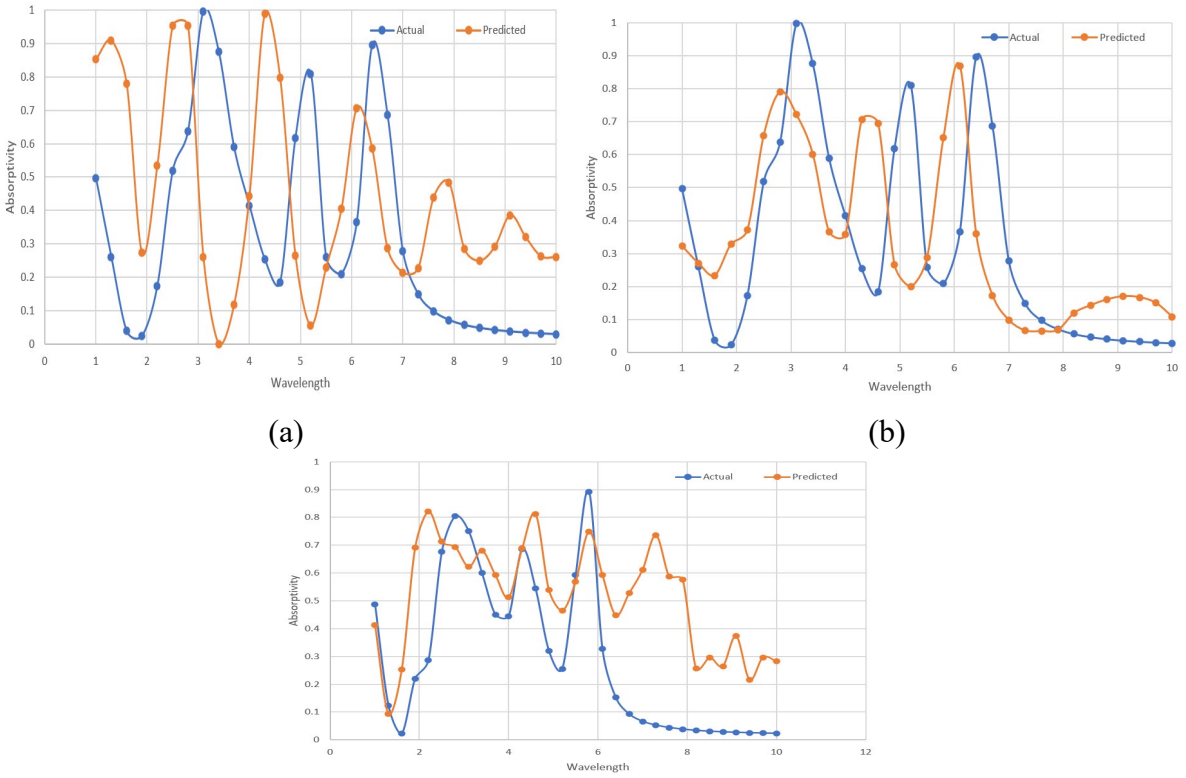


*Fig.5 Comparison of the forecasted and actual absorptivity value for (a)LM at DC = 7.8 and LT =0.002, (b) SCG at DC= 7.8 and LT = 0.002 (c) BR at DC=6.8 and LT=0.002*

## Conclusions

Designing metamaterial and to have desired process is a iterative process which requires time and money. Simulation of these type of materials also requires huge computing power and the validation of simulated result is another hurdle. The rise of ML has given another approach for designing these type of materials. We have simulated and validated a model metamaterial which is capable of absorptivity up to 1 using COMSOL Multiphysics to create a data set for our NARX NN training.

We have used three different training algorithms and found that BR algorithm has predicted the absorptivity most accurately for wavelength value of upto 6 μm after which it has given somewhat noisy results. SCG has been able to capture the absorptivity level more accurately in the later half of wavelength i.e after 6 μm.

The results demonstrate that the NARX NN is effective in predicting the absorptivity behaviour of the designed metamaterial. However, like any ANN, the accuracy of the predictions is heavily influenced by the amount of training data available. To improve prediction accuracy, increasing the size of the training data set would be beneficial.

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