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Prediction of Characteristics Using a Convolutional Neural Network Based on Experimental Data on the Structure and Composition of Metamaterials

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Abstract This work proposes an algorithm for properties predicting metamaterials depending on their structure, physical properties of the components of metamaterials, and their characteristics. In this context, the term "properties" means the result of interacting with the irradiation of a material with electromagnetic exposure of a certain frequency or spectral composition to determine the transmittance/reflection coefficients of the metamaterial.
The model is based on the construction of metamaterial in form of a 3D object, the presentation of physical properties in the form of additional components in the object's vectors, the presentation of experimental data in the form of polynomial coefficients, or the points on the chart of dependencies. Despite the small amount of data, a sufficiently small error rate was obtained for both cases, and the prediction results of experimental data are presented. The amount of experimental data can be increased by supplementary parameters which characterize the conditions under which the experimental data were obtained - polarization, angle of incidence, the intensity of irradiation, etc.
The main issues may arise during the preparation of data for neural network learning due to difficulties in converting 3D formats into the required array of data and taking into account all the circumstances, dielectric and magnetic permeabilities, and specific conductivity.

Keywords metamaterial, 3D convolutional neural network, physical properties of material

AMS 2010 subject classifications 68T07

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1. Introduction

Metamaterials are artificial materials, which properties and structures, usually, have not been observed in nature. The creation of metamaterials is an important breakthrough because they make it possible to obtain properties that are difficult or impossible to obtain naturally [1]. The theoretical design of metamaterial properties is not an easy task, since the exact calculation of all physical interactions takes a large amount of time and energy [2]. Using approximate methods of calculating physical quantities, we gain in time and energy but lose in accuracy. One such approximate method is neural networks. This paper presents an idea and model for predicting the physical characteristics of metamaterials, based on their structure, physical properties of individual components, and measurement conditions.

2. Main idea

In all studies of metamaterials, there is a structure of the material - with all topological characteristics of surface microreliefs or special microstructures as well as the materials that were used; the measurement data: dependence

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graphs, spectra, the measurements conditions, etc. That is, there is a direct relationship: input data - the structure of the material, its composition, and experimental conditions; the initial data are the results of an experiment. In this case, the neural network can be used as a predictive logic circuit. To train a neural network, a sample of various metamaterials with their characteristics (experimentally obtained) is used, and then, based on one component of the sample, we can predict another component [3, 4, 5]. Various methods of such approach are presented in [6, 7, 8, 9, 10, 11]. In the future, there is also an opportunity to use this algorithm for various predictive systems of artificial intelligence [12].

3. Requirements for the procedures

The main problems are derived from the requirements of a neural network itself. This means that in order for a neural network to successfully perform its function, some sufficient conditions must be met, which in the process of research and testing may change depending on the progress of prediction (error function behavior) [13]. The first requirement is data uniformity. This means that the dimensions of structures, the conditions of research, and the scalability of input and output parameters must have the same order. The second requirement is the sample size, that is, the number of training cycles to which a neural network will realize successful training. To form a sample, a large number of experiments with real data obtained in the same measurement conditions (materials, characteristics, procedures, etc.) are required. The third requirement concerns choosing of optimal configuration of a neural network since each situation requires a different approach (type of neural network, number of layers, number of neurons, hyperparameters, etc.).

4. Data preparation for convolutional neural network

In this work, we present only a small amount of the neural network capabilities that can be used to predict the properties of materials.

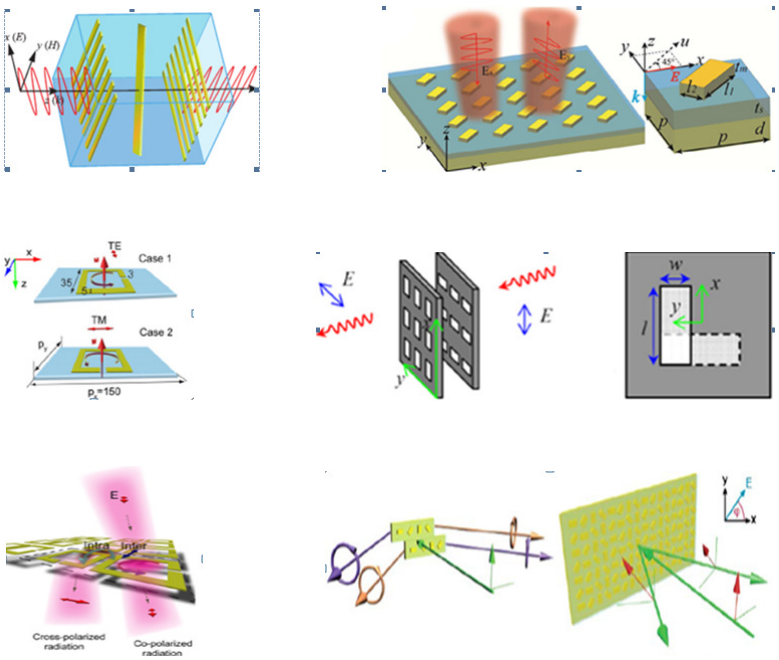


Figure 1. Schematic images of metastructures that were built and used for training a system based on a convolutional neural network [14, 15, 16, 17, 18].

In order to satisfy at least approximately the necessary conditions described above, we use five experimental results of metamaterials measurement (Fig. 1) [14, 15, 16, 17, 18]. Each of them contains data on the structure of metamaterial, the circumstances under which the research was conducted (the angle of incidence of radiation, characteristics of materials, type of polarization), as well as results of the research itself - a functional dependence of transmission coefficient on the frequency of radiation.

5. Dataset structure for the analysis task of metamaterial structure

In this study, a convolutional neural network was used. That is, such a neural network takes as input a tensor that can represent an image. It is difficult to represent the structure of a material using an image, so we used a fourth-rank tensor with three additional channels. Thus, the structure of the material was reproduced using a software package for creating three-dimensional models. Each model was written as a matrix with three columns, where each row is one pixel of a model (coordinates). Three additional channels are the properties of the material that represent this pixel (each set of coordinates (points) has its own properties). That is, we took into account the property of the material, which was fixed for each point separately. In the end, we have an input of 6 channels, where the first three are coordinates of the point, and the last three are the properties of the material at this point, represented by an array

$$X = [x,\, y,\, z,\, \varepsilon,\, \chi,\, \sigma], \tag{1}$$

where x, y, z are the 3D coordinates, ε is the dielectric constant, χ is the magnetic susceptibility, and σ is the conductivity.

The material properties were encoded using digital pixel painting. Each point has been colored, which means it has three additional numbers - RGB: the amount of red, green, and blue shades. Each structure in all metamaterials has its pixels colored to match the real sample, for example, the gold is red, the dielectric is green, etc. Now we need to replace programmatically the color shade numbers with material properties since the colors are not related to the real difference in the properties of different materials. In fact, each color can be replaced by any number of parameters, but in this work, we have taken only three - dielectric constant, magnetic susceptibility, and specific conductivity. The reason for choosing such a set of parameters was the characteristics of metamaterials (transmission coefficient depending on the frequency), which were measured in experimental studies.

6. The procedure for collecting datasets for neural network training

The initial conditions under which experiments were performed, were not included in the input data of the neural network but will be taken into account in future works. In our case, the following were taken as such pre-fixed initial characteristics of the experiment: the angle of inclination of radiation, type of polarization, number of passing plates, and index of refraction of dielectric (all these values were selected due to the fact that the results of the experiment were carried out at different values of these parameters). That is, in this work, the initial measurement conditions are the same for all structures (which were used for the training of the neural networks). Also, various statistical models can be used for research and selection of information for the dataset [19, 20].

7. Type of experimental research

The experimental results were presented in a form of a two-dimensional array, that is, each characteristic was presented as a set of points on a two-dimensional plane. The condition that these data are suitable for our model is that the units of measurement in all characteristics are reduced to a common scale. So, for all graphs, x is the frequency, and y is the pass rate (Fig. 2).

Due to a small amount of required data and a small number of studies, we have eleven material structures and twenty-five graphs of experimental results. The difference in the amount of input and output data is due to the fact

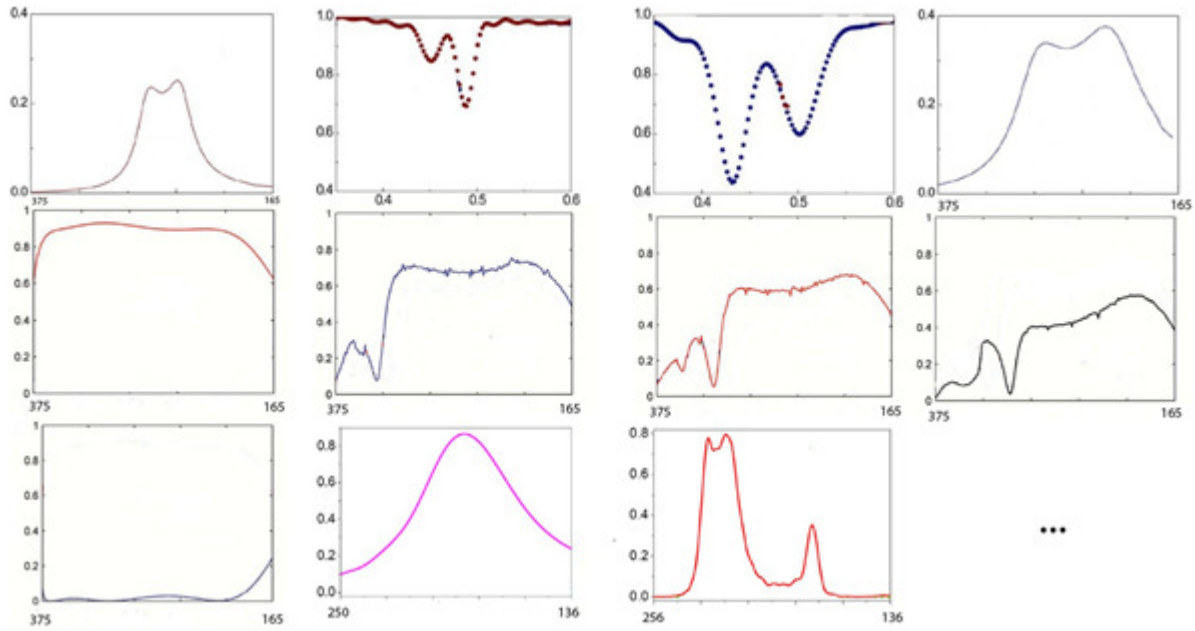


Figure 2. Graphs of experimental studies of the dependence of transmission coefficient on radiation frequency [14, 15, 16, 17, 18]

that the experiments were performed not only for different structures but also, as noted, for different conditions - the refractive index, the angle of inclination of radiation, the number of plates, the type of polarization.

8. Analysis of the problem

To solve such a problem, a neural network is needed, which will be able to learn on 3D models in combination with graphs in which additional parameters are fixed. Thus, in our model, a convolutional neural network was used to process large data sets, namely 3D models [21]. The output neurons will represent parameters that describe each plot of metamaterials experimental studies. That is, for each unique pair: of 3D objects and the measurement conditions, we have unique experimental data in the form of a graph (in our case). By training a neural network in this way, we obtain a model for predicting the parameters of metamaterials. Of course, for a truly effective model for predicting the properties of an unexplored or unknown metamaterial structure, a sufficient amount of ready-made information about existing structures and materials is required. It is also necessary to take into account the originality of each experiment since the main thing is that values that influence the result of an experiment are taken into account, and those that do not influence (or have little influence) are not. The general formula for calculating output value given input values

$$[N,\, Cin,\, H,\, W,\, D]$$

and initial values

$$[N,\, Count,\, Dout,\, Hout,\, Wout]$$

[22] have the following form:

$$out(N_i,\, C_{out,j}) = bias(C_{out,j}) + \sum_{k=0}^{C_{in}-1} weight(C_{out,k}) * input(N_i, k) \tag{2}$$

where $*$ is 3D convolution, N is batch size, C is number of channels, H is height in pixels, W is width in pixels, and D is depth in pixels.

The formulas used to calculate the output array [22] are the following:

$$\begin{aligned} D_{out} &= \left[\frac{D_{in} + 2 \times padding[0] - dilation[0] \times (kernel\_size[0] - 1) - 1}{stride[0]} + 1 \right] \\ H_{out} &= \left[\frac{D_{in} + 2 \times padding[1] - dilation[1] \times (kernel\_size[1] - 1) - 1}{stride[1]} + 1 \right] \\ W_{out} &= \left[\frac{D_{in} + 2 \times padding[2] - dilation[2] \times (kernel\_size[2] - 1) - 1}{stride[2]} + 1 \right] \end{aligned} \tag{3}$$

where padding is indentation (in our case, by default 0), dilation is the distance between kernel elements, kernel_size is the size of the collapsed kernel, more details in PyTorch documentation for 3D convolution.

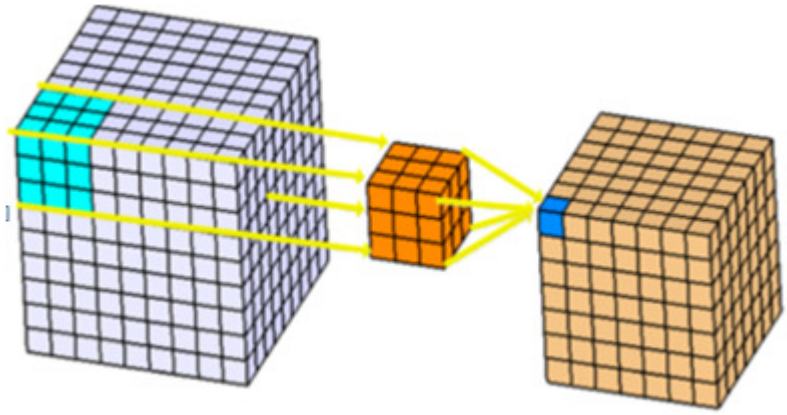


Figure 3. Schematic view of the 3D convolution process

9. Neural network architecture and data processing

The architecture is presented in form of a learning graph or learning model, as shown in the following work figures. For forecasting, two approaches were used to present the graphs - in form of polynomial coefficients and points on a graph. In the first variant, operations were performed to present the graph in form of a functional polynomial of the corresponding order. Fifth-degree polynomial was chosen. With the increasing degree of a polynomial, the appearance of the graph, which approximates the experimental graph, almost does not change. Graph points were scaled to [0, 1]. A schematic view of the algorithm for the first case is presented in fig. 4.

In the second case, a small number of points were taken, which fully describe all the required changes on the experimental graph. The data preparation for the neural network takes place in the following stages:

- Since a huge number of points is difficult to predict, the interpolation is needed to reduce the number of points (in our case to ten);
- In order for a neural network to process data more easily, we scale data to the values from the interval [0, 1]:

$$\max \min \textit{(scale)} = \frac{x - \min(x)}{\max(x) - \min(x)}. \tag{4}$$

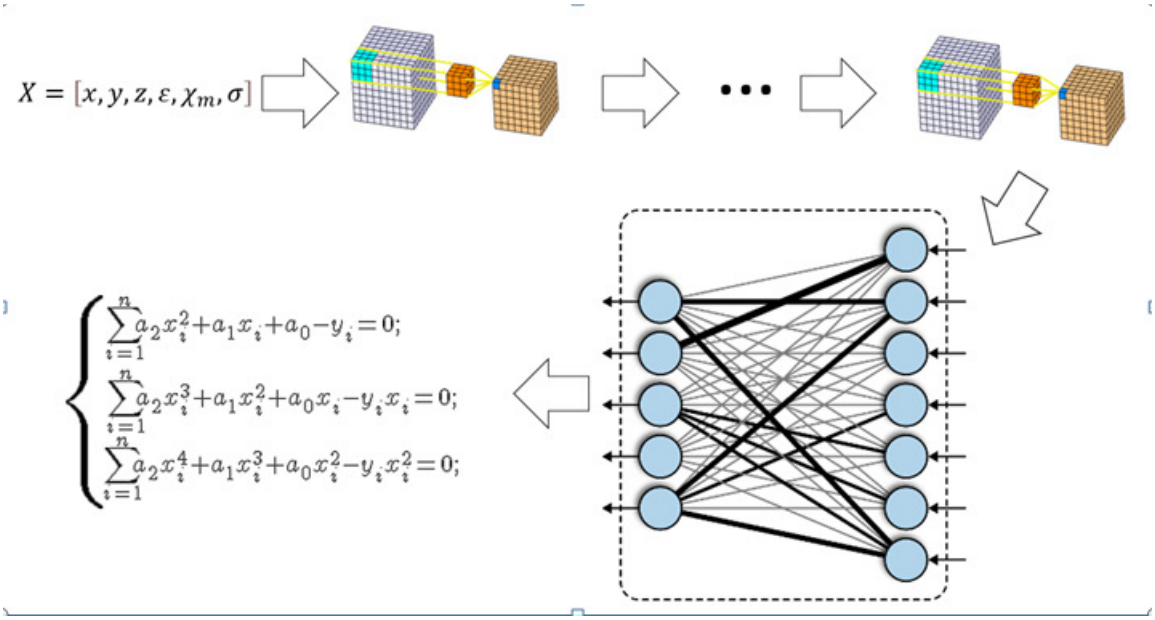


Figure 4. Schematic view of algorithm for case of presenting experimental studies in form of polynomial coefficients

The following figure shows which points were selected as a result of interpolation of graph values:

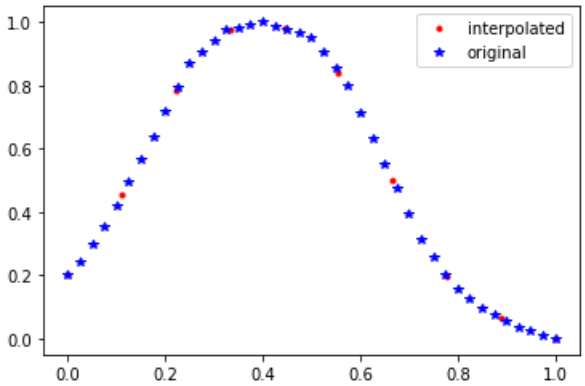


Figure 5. An example of interpolation of values on graph to reduce number of output neurons

The input is a representation of 3D structure of metamaterial and composition of metamaterial (which is represented as three channels with numbers that are attached to each pixel - coordinates). The schematic view of algorithm for the second case is presented in Figure 6.

Using the preselected parameters: $learning\ rate = 1e-3, batch\_size = 1, optimizer = NAdam$, we obtain the following.

10. Results

In the case of graphs presentation in the form of points at the output of the neural network, we have:

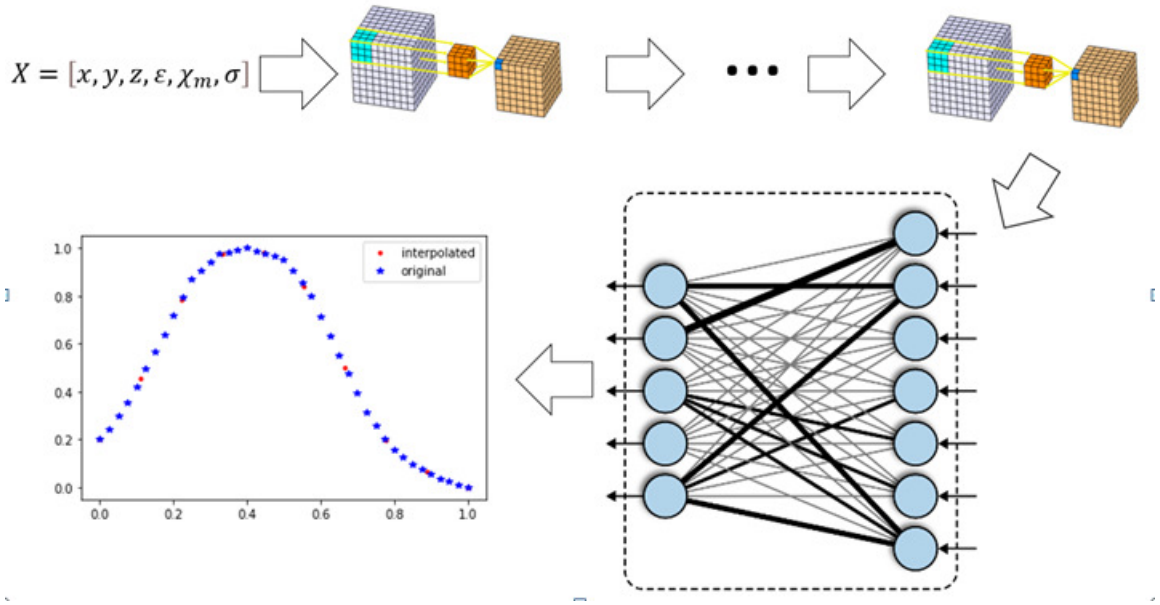


Figure 6. Schematic view of algorithm for case of presenting experimental studies in form of polynomial coefficients

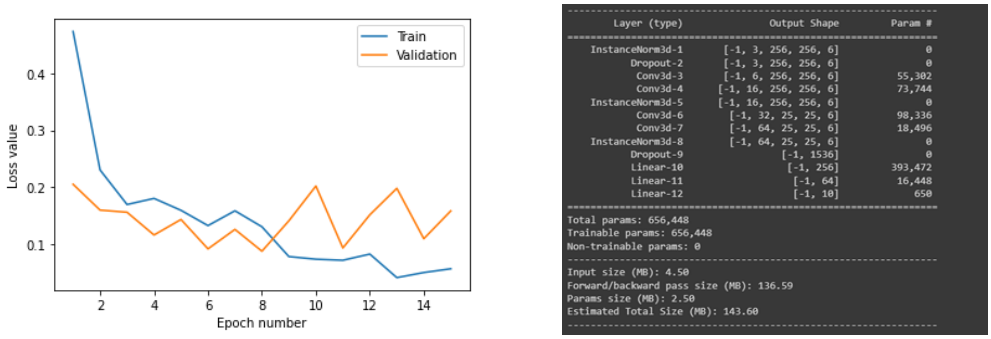
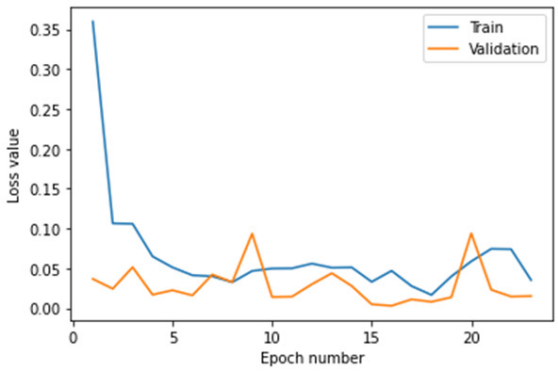


Figure 7. Error dependence on number of training epochs (left) and the learning model in the program window (right) for the first case

Now consider the case with presentation of graphs in the form of polynomials of fifth degree. As one can see from graph (Fig. 9), the system really works and learns, and there have place error decrease with each subsequent learning epoch. And therefore, with each subsequent epoch, the prediction of output graph will be more and more qualitative and plausible. Of course, the graphs will not completely coincide for a number of reasons - a small amount of data; insufficient information about real influence of all factors on measurement of experimental data; not ideal conversion of software 3D package from software formats (ply, obj, fbx ...) to xyzrgb; conversion of rgb channels into channels with physical properties; scaling of graphs to a unit interval, non-ideality of neural network architecture - hyperparameters, number of layers, number of neurons, etc. Despite this, we have obtained a neural network that can be improved and an algorithm that makes it possible to analyze and predict properties and structure of metamaterials.

Despite the fact that the error for the case with polynomials is not very big, the difference between required and predicted coefficients is huge due to the fact that when error increases even by a small fraction, coefficients change to an incomparably greater degree, so this option is not very effective in comparison with the option of graphs representation in point form. As a result, we obtained a sufficiently high-quality model for predicting the characteristics of unknown metamaterials, as shown in Fig. 11:




```
----------------------------------------------------------------
      Layer (type)               Output Shape         Param #
================================================================
InstanceNorm3d-1          [-1, 3, 256, 256, 6]               0
        Dropout-2         [-1, 3, 256, 256, 6]               0
         Conv3d-3         [-1, 6, 256, 256, 6]          55,302
         Conv3d-4        [-1, 16, 256, 256, 6]          73,744
InstanceNorm3d-5        [-1, 16, 256, 256, 6]               0
         Conv3d-6        [-1, 32, 25, 25, 6]            98,336
         Conv3d-7        [-1, 64, 25, 25, 6]            18,496
InstanceNorm3d-8        [-1, 64, 25, 25, 6]               0
        Dropout-9                 [-1, 1536]               0
        Linear-10                  [-1, 256]         393,472
        Linear-11                   [-1, 64]          16,448
        Linear-12                    [-1, 5]             325
================================================================
Total params: 656,123
Trainable params: 656,123
Non-trainable params: 0
----------------------------------------------------------------
Input size (MB): 4.50
Forward/backward pass size (MB): 136.59
Params size (MB): 2.50
Estimated Total Size (MB): 143.59
----------------------------------------------------------------
```

Figure 8. Error dependence on number of training epochs (left) and the learning model in the program window (right) for the second case

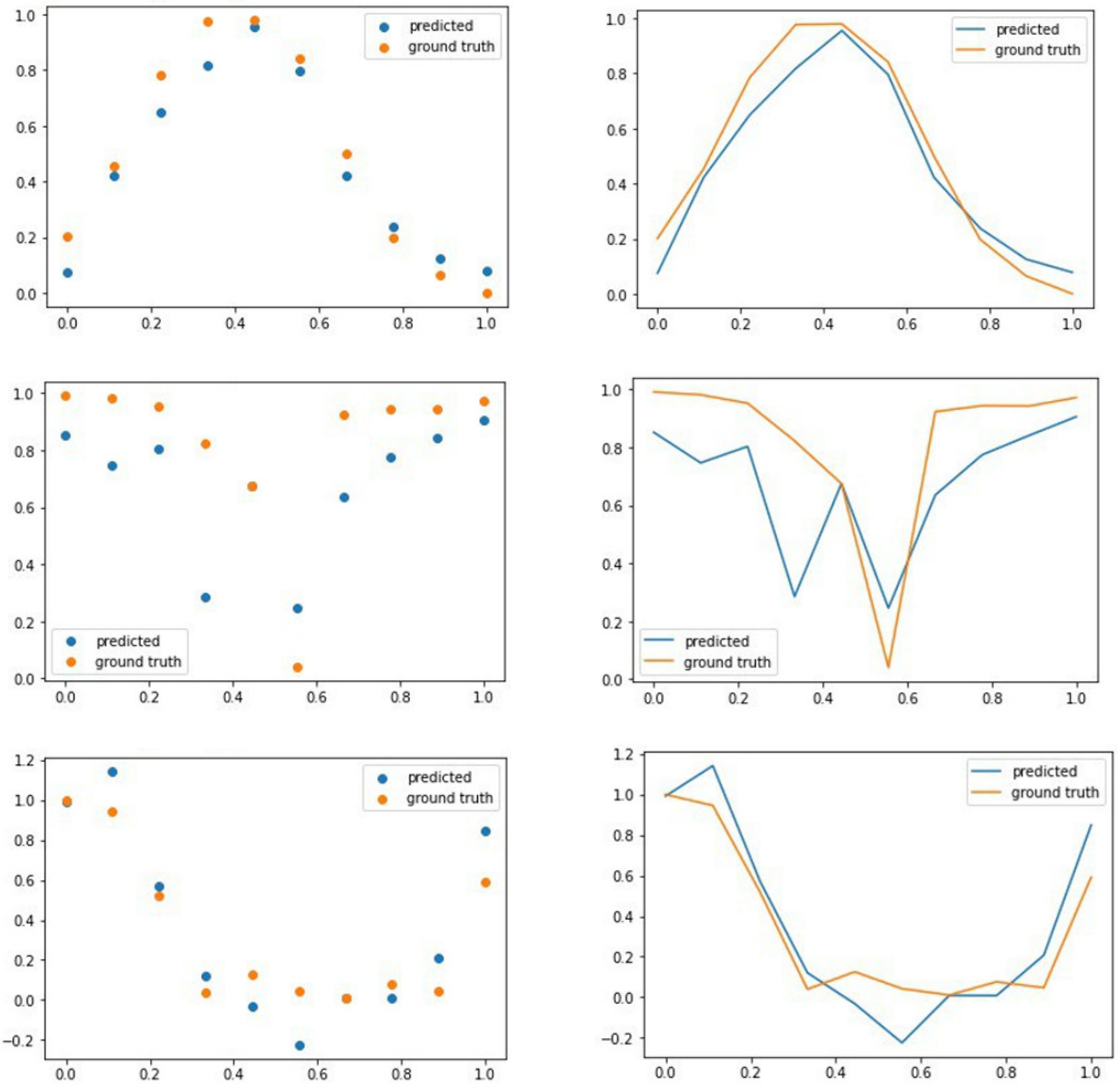


Figure 9. Real characteristics and predicted based on presented model

On X-axis, the values are scaled due to the needs of neural network architecture, but this does not affect the result itself. Analyzing the obtained results, we can summarize the following - the very nature of predicted characteristics is preserved, which means that we got a system that was developed in the right way; of course, the number of points does not allow us to fully obtain the desired result, which is associated with the increasing complexity of calculations with an increasing number of points; a considerable error is due to a very small amount of data and the complexity of data preparation algorithm for neural network, which means that a large number of inaccuracies accumulation can give a large error.

11. Conclusion

This work presents an idea and a model for predicting the properties of metamaterials based on experimental studies of these structures. It was shown how the main properties and differences of structure can be obtained and converted digitally and how they need to be converted to the format required by neural networks. The paper uses the main advantages of a convolutional neural network for 3D objects. It is shown that even with a small amount of data and a large number of nuances that can affect the quality of results, sufficiently small errors were obtained for two cases - presentation of experimental graphs in form of polynomial coefficients and points on the graph. The main points that need to be paid attention to when using this algorithm and difficulties that may arise in the development of similar systems are analyzed.

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REFERENCES

1. N. I. Zheludev, *The Road Ahead for Metamaterials*, SCIENCE, vol. 328, pp. 582–583, 2010.
2. M. Maasch, *Tunable Microwave Metamaterial Structures*, Springer Theses, Schweiz, 2018. DOI: 10.1007/978-3-319-28179-7.
3. H. P. Fischer, *Convolutional Neural Network Surrogate Models for the Mechanical Properties of Periodic Structures*, J. Mech. Des., vol. 142, 142(2): 024503, 2020. DOI: 10.1115/1.4045040.
4. G. B. Goh, N. O. Hodas, A. Vishnu, *Deep learning for computational chemistry*, Wiley Periodicals, Inc., vol. 38, pp. 1291–1307, 2017. DOI: 10.1002/jcc.24764.
5. S. Kadulkar, Z. M. Sherman, V. Ganesan, T. M. Truskett, *Machine learning-assisted design of material properties*, Annual Review of Chemical and Biomolecular Engineering, vol. 13, pp. 235–254, 2022.
6. Y. Xu, X. Zhang, Y. Fu, Y. Liu, *Interfacing photonics with artificial intelligence: an innovative design strategy for photonic structures and devices based on artificial neural networks*, Photonics Research, vol. 9, pp. B135–B152, 2021.
7. O. Khatib, S. Ren, J. Malof, W. J. Padilla, *Deep Learning the Electromagnetic Properties of Metamaterials – A Comprehensive Review, Advanced Functional Materials*, Advanced Functional Materials, vol. 31, 2101748, 2021.
8. J. Jiang, M. Chen, J. A. Fan, *Deep neural networks for the evaluation and design of photonic devices*, Nature Reviews Materials 6, pp. 679–700, 2021.
9. J. Kabir, Y. Wang, M. Yu, Q. J. Zhang, *Neural Network Inverse Modeling and Applications to Microwave Filter Design*, IEEE Transactions on Microwave Theory and Techniques, vol. 56, no.4, pp. 867–879, 2008.
10. Z. Liu, L. Raju, D. Zhu, W. Cai, *A Hybrid Strategy for the Discovery and Design of Photonic Structures*, IEEE Journal on Emerging and Selected Topics in Circuits and Systems, vol. 10, no.1, pp. 126–135, 2020.
11. I. Malkiel, M. Mrejen, A. Nagler, *Plasmonic nanostructure design and characterization via Deep Learning*, Light: Science&Applications 7, 2018. DOI: 10.1038/s41377-018-0060-7.
12. Y. Yakimenko, S. Stirenko, D. Koroliuk, Y. Gordienko, F. M. Zanzotto, *Implementation of Personalized Medicine by Artificial Intelligence Platform*, Statistics, Advances in Intelligent Systems and Computing (AISC), vol. 1428, pp. 597–611, 2016. DOI: 10.1007/978-981-19-3590-9_46.
13. I. Goodfellow, Y. Bengio, A. Courville, *Deep Learning*, The MIT Press, 2016. DOI: 10.1063/1.4939564.
14. L. Cong, Y. K. Srivastava, R. Singh, *Inter and intra-metamolecular interaction enabled broadband high-efficiency polarization control in metasurfaces*, Appl. Phys. Lett. 108, 2016. DOI: 10.1063/1.4939564.
15. F. Ding, Z. Wang, S. He, V. M. Shalaev, A. V. Kildishev, *Broadband High-Efficiency Half-Wave Plate: A Supercell-Based Plasmonic Metasurface Approach*, ACS Nano, 9, 4, pp. 4111–4119, 2015. DOI: 10.1021/acsnano.5b00218.

16. C. Huang, *Efficient and broadband polarization conversion with the coupled metasurfaces*, Optics Express, vol. 23, issue. 25, pp. 32015–32024, 2015. DOI: 10.1364/OE.23.032015.
17. A. Shaltout, K. Liu, A. Kildishev, V. Shalaev, *Photonic spin Hall effect in gap–plasmon metasurfaces for on-chip chiroptical spectroscopy*, Optica, vol. 2, issue. 10, pp. 860–863, 2015. DOI: 10.1364/OPTICA.2.000860
18. N. K. Grady, J. E. Heyes, D. R. Chowdhury, M. T. Reiten, A. K. Azad, A. J. Taylor, D. A. R. Dalvit, H. T. Chen, *Terahertz Metamaterials for Linear Polarization Conversion and Anomalous Refraction*, Science, vol. 340, pp. 1304–1307, 2013. DOI: 10.1126/science.1235399.
19. D. Koroliuk, V. S. Koroliuk, E. Nicolai, P. Bisegna, L. Stella, N. Rosato, *A statistical model of macromolecules dynamics for Fluorescence Correlation Spectroscopy data analysis*, Statistics, Optimization and Information Computing (SOIC), vol. 4, pp. 233–242, 2016. DOI: 10.19139/soic.v4i3.219.
20. S. O. Dovgyi, O. I. Yurikov, M. O. Zozyuk, *On One Statistical Model of Error Rate in the Stream of Packet Data Transmission through Communication Channels*, Cybern. Sys. Anal., vol. 56, pp. 739-–744, 2020. DOI:10.1007/s10559-020-00294-x.
21. V. Sze, Y. H. Chen, T. J. Yang, J. Emer, *Efficient Processing of Deep Neural Networks: A Tutorial and Survey*, Proceedings of the IEEE, vol. 105, pp. 2295–2329, 2017. DOI: 10.1109/JPROC.2017.2761740.
22. https://pytorch.org/docs/stable/generated/torch.nn.Conv3d.html#torch.nn.Conv3d, *Applying a 3D convolution*, PyTorch Contributors, 2022.