Application of Neural Network Method to Restore the Refraction Index of Homogeneous Dielectric Layer

Dmitry N. Tumakov and Diana M. Khairullina
Kazan Federal University, Kremlevskaya Street 18, Kazan, Russia

Abstract: The research studied the problem of a homogeneous layer refraction value recovering by Neural Network Method. The case with the known thickness is studied. We used three neuron activation functions: a linear, a sigmoidal and Gauss function. The network training is conducted by two methods: the method of back propagation and genetic algorithm. The desired value of refraction index is chosen as the average one between the results of independent neural networks trained according to the same initial data. This approach makes sense because the target functions of networks comprise the plurality of local extrema and each new network with a random initial vector of weights provides different but close results. The method of cross validation estimarted the accuracy of refractive index recovery for different activation functions and the methods of network training. The conclusion that the genetic algorithm provides better results than the gradient methods (in particular, the method of error backpropagation). It was shown that the number of neurons increase leads to a natural improvement of recoverable values accuracy for refractive index. The "best" objective functions are obtained for neural networks with sigmoidal and Gaussian activation function. It is expressed by more sustainable behavior of error at continuous change of other network settings. The plots of error dependence for the recovery of the refractive index on the sample size and the number of neurons are presented which confirm the findings.

Key words: Refractive index recovery, neural networks, genetic algorithm, Gaussian, local extrema

INTRODUCTION

For the development of laminated coating technologies and the testing of layers during production as well as for a wide range of applications encountered in optics and electrodynamics, the restoration of the refractive indices of layered structures is often required. The restoration of one dimension refractive index profile for a layer is an inverse problem and is one of the most important tasks within this field. Finding of an unknown profile may be carried out on the basis of various data such as the coefficients of the reflected or transmitted field, an input impedance, the scattered electric or magnetic fields. During the restoration a profile may be represented as a laminate one or as a continuous one (Emad *et al.*, 2009).

During the solution of profile reconstruction issues two approaches are used: the methods in the time domain (Li and Li, 2008; Rahman and Marklein, 2009) and the methods in the frequency domain. The methods in the time domain require a rather complex and high-precision equipment for the generation and the registration of short pulses which complicates the use of these methods in practice. Often the terahertz pulsed spectroscopy is used

(Zaytsev *et al.*, 2013, 2014). The methods in the frequency domain determine the required measurement parameters at different frequencies and at multiple angles of incidence and different polarization of waves. The dielectric permeability (or the refractive index) is approximated by truncated series or presented as a set of individual values (Semnani and Kamyab, 2009; Pleshchinskii and Tumakov, 2012).

The resulting inverse problems during profile reconstruction are ill-conditioned and their solutions demand the methods of regularization. These methods provide a stable but they affect the accuracy. The error of methods in the frequency domain depends on the choice of a frequency band used in the inverse problem of Pleshchinskii and Tumakov (2013) and Tumakov (2014). However, the precise criteria for the selection of the frequency range are not always easily predictable (Lin *et al.*, 2011). Any a priori information is important for inverse problems solution. Such information may be obtained for example, during the analysis of the amplitude-frequency characteristics. For example, the passage of the waves through the gradient layers of certain types (Anufrieva *et al.*, 2013), the fractal layers (Anufrieva *et al.*, 2014) or stratified geologic

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Corresponding Author: Dmitry N. Tumakov, Kazan Federal University, Kremlevskaya Street 18, Kazan, Russia

environments (Kipot and Tumakov, 2014). It is also necessary to bear in mind that sometimes certain measured values at different frequencies are the same for different layers (Anufrieva and Tumakov, 2012).

Among the methods of solutions one may distinguish analytical approximation techniques (Ahmad *et al.*, 2006; Casagranda *et al.*, 2006; Mertzanides *et al.*, 2000) and the methods of consistent effect removing of the overlying layers (layer stripping techniques) (Hashish, 2003; Caviglia and Morro, 2007). Most often, the issues of profile restoration are solved by optimization techniques which minimize the error between the measured and calculated data. Also, the problems arise when the data are incomplete or corrupted by noise (Nakhkash *et al.*, 1999).

The used methods may be divided into the methods of local and global optimization. For example, the methods of local optimization are the gradient and quasi-Newton methods as well as the Gauss-Newton Method (Abubakar *et al.*, 2006; Haber *et al.*, 2007). These methods are fast but often converge to local minima caused by the non-linear nature of a problem. Therefore, these approaches may be recommended when a priori information is known. A priori information is not needed for global optimization methods but they require a large number of iterations.

From the global optimization methods used in inverse problems of electrodynamics, we may distinguish the method of neural networks (Brovko *et al.*, 2008), the genetic algorithms (Caorsi *et al.*, 2001; Chiu and Chen, 2000) and the particle swarm optimization techniques (Donelli *et al.*, 2009; Huang and Mohan, 2005; Huang *et al.*, 2008; Emad and Hashish, 2007). Each of these methods has both the advantages and disadvantages of (Van Den Bergh and Engelbrecht, 2006; Samii, 2003; Eberhart and Shi, 1998). Because of this, sometimes we use different methods of hybrid technology to take advantage of each of the methods by Wei *et al.* (2007) and Franceschini *et al.* (2006).

In the present research to restore the profile the method of neural networks was used. It is worth noting that now a days neural networks are proven to be a powerful and an effective tool for complex process modeling in many areas of science (Haykin, 2009). On the basis of functioning and the principle of biological neural network operation one may recreate an artificial neuron model with a hardware and a software implementation. Artificial Neural Networks (ANN) are gaining popularity due to the relative simplicity of the structure and the possibility to adapt to the specific range of tasks. It is worth to take into account ANN applicability is determined, primarily from the context of the set task.

ANN training is rather complicated and time-consuming process. There are many different learning algorithms which have their pros and cons (Schmidhuber, 2015). Among the algorithms the backpropagation method may be mentioned primarily which is the gradient method and accordingly is well suited for the tasks with a distinct global extremum. For the class of problems with the plurality of local extrema, the global optimization such as genetic algorithm are more preferred ones.

In this research, ANN training is conducted by two methods: the method of error back propagation and genetic algorithm. The conclusion of unfitness to this class of problems of a error backpropagation method in particular and the gradient methods in general.

The errors of the desired refractive index for a layer are estimated for three activation functions: piecewise-linear, sigmoidal and Gauss function. It was concluded that the slightly better results are provided by ANN with Gaussian activation function. There numerous plots of neural network error dependence on the number of training data are presented.

PROBLEM SET

Let a plane harmonic electromagnetic wave $u_0(x, t) = A_0 \exp\{-ik_0 n_1 x + i\omega t\}$ falls on a uniform layer with thickness L and an unknown refractive index n_2 (Fig. 1). Here A_0 is the wave amplitude, k_0 is the vacuum wave number, n_1 the refractive index of the first medium, ω is the frequency of the wave distribution. In the unknown functions, let's move from the variable t to ω, so all functions will depend on the variables x and ω. The value shall be restored n_2 using the known elements of reflected wave $u_1(x, \omega)$ and passed wave $u_3(x, \omega)$, measured at a fixed frequency ω.

The problem will be solved by the method of neural networks. It is necessary to consider two methods of network training: the method of backpropagation and the
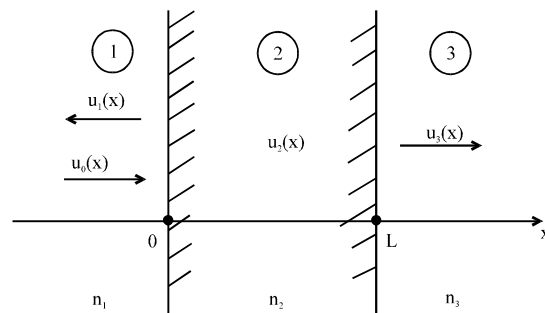

Fig. 1: The issue geometry

genetic algorithm using the three most common activation functions: a piecewise-linear, a sigmoidal and a radial (Gaussian function) one.

NEURAL NETWORKS

Each neuron is a unit that receives a signal from a previous layer and transmits a signal to the next one. The function calculating the output signal of an artificial neuron is called activation function. As an argument, the function takes the signal obtained at the output of a so-called adder which represents the sum of weight products and the values of input neurons. The weights may be considered as some channels that characterize the strength of the link between neurons and simulating the work of biological synapses. Thus, the ANN may be represented as a set of simple elements, the neurons performing the processing of input data followed by the issuance of the resulting value. The block diagram of a two-layer ANN is shown by Fig. 2.

The most widely used activation functions are the linear, sigmoid and radial one as well as some modified versions of these functions. The correctly chosen activation function in conjunction with the learning algorithm greatly improves the convergence of a neural network. Therefore, on the basis of the experiments performed, it is necessary to choose the best option for a particular task solution. The output neuron signal with a linear activation function is equal to the combined input, i.e., the output of the adder:

$$S_i = \sum_{j=0}^{N} w_{ij} x_j$$

Where:
w_{ij} = The neuron network weights
x_j = The inputs in the ith neuron of the current layer

Here, w_{io} the threshold value, $x_o = 1$. Piecewise linear functions (Fig. 3) are used most commonly:

$$f(S) = \begin{cases} 1 & S > 1/a, \\ aS & 0 \le S \le 1/a, \\ 0 & S < 0 \end{cases}$$

The derivative of a linear function is equal to the slope line ratio:

$$f'(S) = \begin{cases} 0 & S > 1/a, \\ a & 0 \le S \le 1/a, \\ 0 & S < 0 \end{cases}$$

The piecewise linear functions are the ones of the easiest activation functions and are easily implemented in
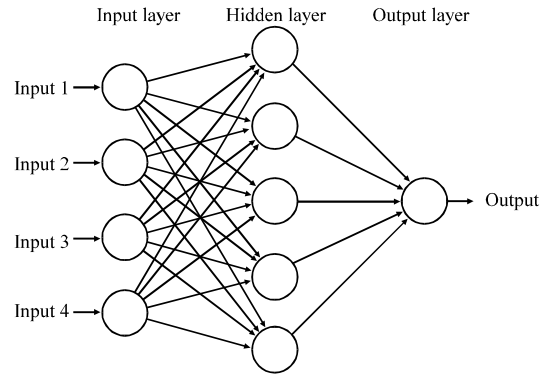

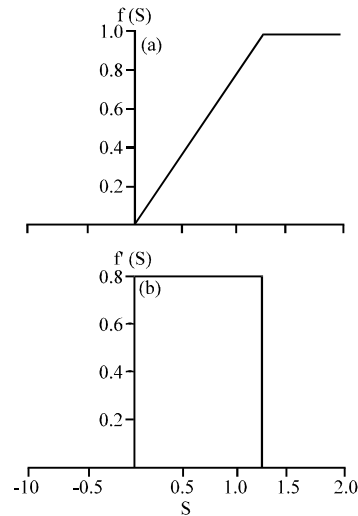Fig. 2: A two-layer model of an artificial neural network

Fig. 3: Piecewise linear activation function ($\alpha = 0.8$) and its derivative

practice. However, these functions have a significant drawback their derivative has a discontinuity and the gradient methods can not be used to train ANN of this type.

The unipolar sigmoid activation function varies in the range from 0-1 (Fig. 4) and is described by the following formula:

$$f(S) = \frac{1}{1 + e^{-\alpha S}}$$

The distinguishing feature of a sigmoid function is its monotony and differentiability on the whole definitional domain as well as a simple expression of its derivative:

$$f'(S) = \alpha f(S)[1 - f(S)]$$

which may be used in the gradient training algorithms. A separate ANN class includes the network of radial basis
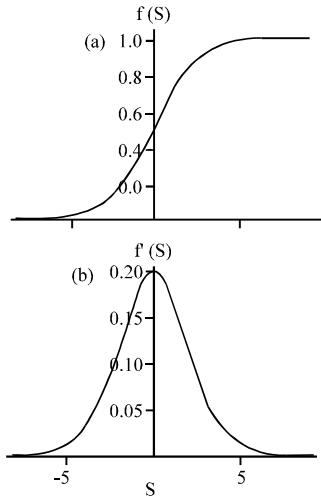
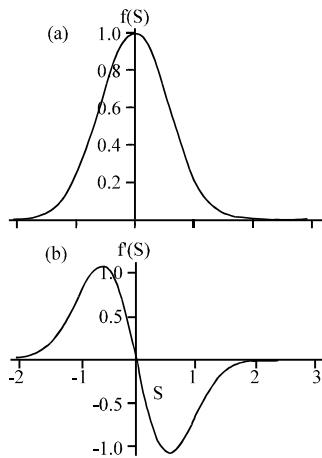Fig. 4: Sigmoid activation function (α = 0.8) and its derivative

Fig. 5: Gaussian activation function and its derivative

functions that use radial basis functions as activation functions. This function may be a Gaussian function (Fig. 5):

$$f(S) = e^{-\frac{S^2}{\sigma^2}}$$

where the parameter σ is a material number. The Gaussian function derivative is expressed by the formula:

$$f'(S) = -\frac{2S}{\sigma^2} f(S)$$

and also has a simple representation as well as the derivative of sigmoid function. Having defined a neural network structure one should find the values of the weights w_{ij} and thethresholds w_{i0} to minimize the error at the output of a neural network. To solve this problem the training algorithms are used. Let's consider some of them.

The most famous teaching method is the error backpropagation (backpropagation algorithm). The basis of this algorithm is the method that computes the gradient vector for further process of weight refinement. The vector direction corresponds to the shortest descent on the error surface. The local minima and the choice of step length have certain difficulties. The differentiability of activation function determines the possibility of using the method of back-propagation. This method involves the training with a "teacher", i.e., the learning sample on which the network will be trained, it contains the input data and the desired response to them which may be represented as the vectors $X = x_1,...,x_m$ and $D = d_1,...,d_n$, respectively. By comparing the actual and target (desired) values the error of learning is calculated on the basis of which based ANN efficiency as a whole is estimated. From these differences the error vector $E = e_1,...,e_n$ is generated, the size of which coincides with the dimension of the vector output signals $Y = y_1,...,y_n$.

At each step of learning the jth weight of the ith neuron is specified by the Delta rule which may be written as follows:

$$w_{ij}(t+1) = w_{ij}(t) + \eta e_i x_j$$

The signal number j varies from one to the dimension of an input vector m. The neuron number varies from one to the number of neurons. The magnitude t the number of the current practice iteration, η the speed of network practice. The input neuron weight error number decreases proportional to the total neuron error.

The use of a sigmoidal activation function has allowed to extend the range of tasks and operate with continuous signals but required the modification of the learning algorithm. The amended version is aimed at minimizing the mean square error function:

$$\delta = \frac{1}{2}\sum_{i=1}^{n} e_i^2 = \frac{1}{2}\sum_{i=1}^{n}(d_i - y_i)^2 \qquad (1)$$

This function is defined by the matrix of weight ratios w_{ij}, where i is the neuron number and j is the input number into ith neuron. The ultimate goal of practice is the obtaining of the global minimum δ. In order to implement this task, you may use the method of gradient descent followed by the adjustment of weights in the direction of a surface antigradient:

$$\Delta w_{ij} = -\eta \frac{\partial \delta}{\partial w_{ij}}$$

Let's calculate the partial derivatives and we obtain the following:

$$\Delta w_{ij} = \eta (d_i - y_i) f'(S_i) x_j$$

Note that when you use the Delta rule the activation function must be continuously differentiable within the entire domain.

Now let's consider the method of global optimization the genetic algorithm. The genetic algorithm is the method that reflects the natural evolution of the desired solution. It uses an evolutionary principle of survival for the most suitable species. The optimization occurs by crossover and the mutation of chromosomes $W = \{w_{ij}\}$ of this population. The chromosome W is represented by a series of genes w_{ij} which may be encoded as a vector (of a "genotype"). It is assumed that a genotype has a fixed length. Let's note that there are variants of the algorithm, free from this limitation. During the first iteration a plurality of initial population genotypes is generated randomly. The fitness function δ helps to assess the level of fitness for each individual and to create a new population of individuals on this basis. From the resulting set of solutions called generations, the best individuals are selected based on the value of fitness which again experience the crossover and mutation operations. The descendants should be able to inherit the attributes of both parents.

"Mixing" can be done in different ways. Let's consider the way of crossing in which another gene is chosen randomly with an equal probability from ancestral genes located in the same position. Then the genes of a constructed" chromosome are unlikely mutated by a small amount. The generation of new populations occurs as long as the fitness function is optimized. Thus, the sequence of these iterations may imitate an "evolutionary process".

LAYER REFRACTIVE INDEX RECOVERY

Let's consider the case where the layer thickness L is known. We assume that measurements of the electric and magnetic fields are performed on both sides of the layer. The measurement results may be represented by two complex variables u_1 (0) and u_3 (L). Thus, the projected neural network will comprise four neurons at the input $(Re[u_1(0)], Im[u_1(0)], Re[u_3(L)]$ and $Im[u_3(L)])$ and one output neuron (n_2).

As the result of numerical experiments during ANN training with the sample containing M experiments, we

may conclude that the mean square error δ has many local extrema and the backpropagation method will stay in these local minima. It is obvious that the other gradient methods based on local optimization will behave in a similar way.

So, we abandon the gradient methods and will train the networks by a genetic method. At each ANN training, we get a full set of predetermined weights $W = \{w_{ij}\}$. At that due to the arbitrary starting values $W^{(0)}$ as well as the variability of weight W mutations at each training the weights W will be different. The restoration of the value n_2 will also be varied within some interval. Let's assume that the values n_2 calculated by the neural network approximately satisfies the normal law. Then this will allow to use the following approach. For the same experiments let's carry out the training of the network K times, thus obtaining de facto K of independent ANN. Then let's calculate the following outputs for each network: n_2, $i = 1...K$. The final value will be obtained as the average one:

$$n_2 = \frac{1}{K} \sum_{i=1}^{K} n_{2,i}$$

Let's choose K = 5 for numerical experiments. In order to check the accuracy of the approximation method let's use the cross validation method. Let's use the following modification of the method. Suppose we have M of experiments. Let's choose a single experiment randomly, train the network on the remaining M-1 data. Compare the obtained n_2 with the known values obtaining the approximation error ε_i. Let's perform R of experiments, the result will be the sequence $\varepsilon_1,...,\varepsilon_R$. Let's choose the worst value $\varepsilon = \max_{i=1..R} \varepsilon_i$. Let R = 20, then we can say with the confidence of 95% that the neural network "works" with an error ε. Let's assume that R = 20 for all numerical experiments.

Let's restore the refractive index with a network containing one neuron in a hidden layer. Figure 6 shows the error dependence ε on the number of samples M. It can be seen that the error is quite but more stable and somewhat lower values ε will be for the Gauss function activation (dotted line). It should be that at larger M an error instability occurs, conditioned by a retraining.

The following experiments were conducted for the ANN with three and seven neurons in a single hidden layer (Fig. 7). Obviously, the accuracy improves with the number of neurons increase (and accordingly, the number of weights increase). In these cases, it is difficult to single out any activation function. The example of ANN with seven neurons shows that the network works better at low values and starting from M = 35, ε values begin to increase, especially this effect is visible for a piecewise-linear activation function (solid line).
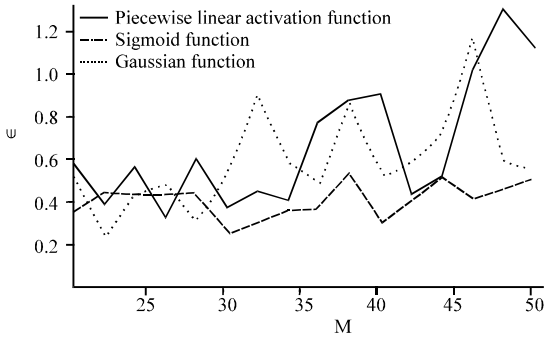
Fig. 6: The dependence of ε on M. ANN: 1 hidden layer with 1 neuron. Solid line piecewise linear activation function, dashed-sigmoid, spot Gaussian function
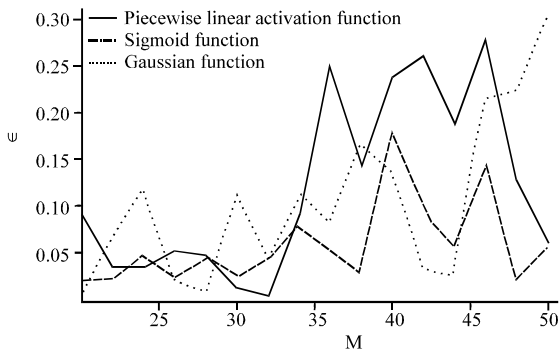

Fig. 7: Dependence of ε on M. ANN: 1 hidden layer with 3 neurons (to the left), 1 hidden layer with 7 neurons (to the right). Solid line piecewise linear activation function, dashed line sigmoid, spot Gaussian function

The confirmation that the number of neurons improves the accuracy can be seen by Fig. 8a. The figures demonstrate the graphs for one neuron (solid line), the dotted line for three neurons and the dotted one for seven neurons. You may also notice that the radial activation function (right figure) provides a more stable accuracy than a sigmoid one (Fig. 8b).

Figure 9 shows the dependence of ε on the number of neurons N of a neuron network with one hidden layer. It can be seen that for sufficiently large values N>12, the error values ε at the increase of N become better and more stable at ε≈0.04.

Let's consider the restoration of the layer refractive index by the field passed. In this case, the neural network will comprise two inputs $Re[u_3(L)]$, $Im[u_3(L)]$ and one output n_2. The restoration will be performed on a multilayer network with sigmoid (solid line on Fig. 10) and radial activation functions (dashed line on Fig. 10).
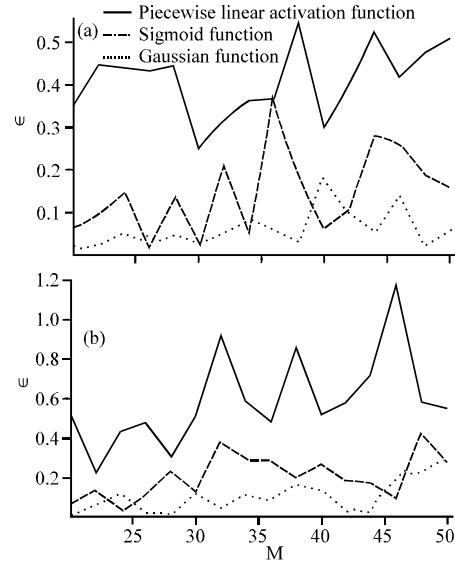

Fig. 8: Dependence of ε on M; a) ANN with 1 hidden layer. Sigmoid activation function; b) Gauss function activation. Solid line 1 neuron, dashed line 3 neurons, dotted line 7 neurons
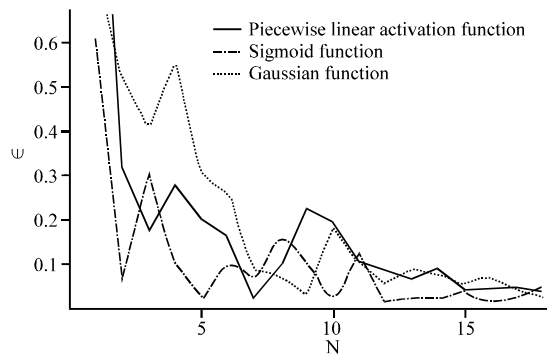

Fig. 9: The dependence of ε on the number of neurons N. ANN with one hidden layer. Solid line piecewise linear activation function, dashed line sigmoid function, dotted line Gaussian function

The recovery results by a two-layer and a three-layer ANN can be considered as close ones. Note that the network consisting of two hidden layers of neurons containing 5 neurons each has only 10 hidden neurons and 40 weights plus 11 thresholds (51 gene in the chromosome). The network, comprising 3 layers with 3 neurons each contains 9 and 27 weights plus 10 thresholds (37 genes). The learning process using a genetic algorithm, depends primarily on the number of weights. It is possible to make a preliminary that the use of multi-layer networks may be preferable from the learning time point of view.
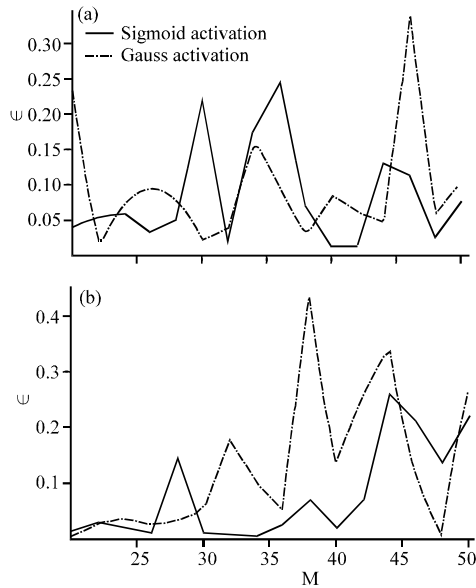
Fig. 10: The dependence of ε on M. The recovery by elapsed field. ANN: 3 hidden layers with 3 neurons in each (to the left), 2 hidden layers with 5 neurons in each (to the right). The solid line is the sigmoid activation function, the dotted line is the Gauss function

SUMMARY

The use of neural network method to restore the refractive index of a homogeneous layer gives quite good results. The use of genetic algorithm for a single-layer neural network training (the number of neurons is >12), guarantees the recovery of the refractive index with an error of <10%. The number of neurons increase leads to the improved accuracy of the network operation.

CONCLUSION

The training of a neural network to restore the refractive index of a homogeneous layer is reasonable to carry out using a genetic algorithm. This conclusion follows from the fact that the objective function (network error) comprises a plurality of local extrema.

The second conclusion is quite obvious that the number of neurons increase improves the approximation of the desired values and the network performance with the increase of its structure complexity (increase of neurons) becomes a more stable one.

The third conclusion regarding the activation functions shows that all functions considered in the research (linear, sigmoid and Gaussian function) are approximately the same and approximate the desired refractive values. But ANN, giving more stable solutions are obtained using a Gaussian function activation.

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