SOLUTION OF INVERSE RADIATIVE TRANSFER PROBLEMS IN TWO-LAYER MEDIA WITH ARTIFICIAL NEURAL NETWORKS

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ABSTRACT

In the present work a hybridization of the Levenberg-Marquardt method (LM) with Artificial Neural Networks (ANN) is used for the solution of the inverse radiative transfer problem in a two-layer medium. The ANNs provides good initial guesses for the LM method. The absorption and scattering coefficients of both layers are estimated using external and internal detectors. Using only external detectors are obtained non unique solutions.

1. NOMENCLATURE

f_j = intensity of the external radiation sources, $j = 1 \ or\ 2$
$f(.)$ = activation function
$\bar{F}$ = vector of residues
$g(.)$ = activation function
I = intensity of the radiation
J = Jacobian matrix
k_{a_i} = absorption coefficient, $i = 1 \ or\ 2$
L_i = thickness of the layers, $i = 1 \ or\ 2$
l_k = difference between the estimates t_k and the exact values Z_{kexact}
N = total number of experimental data
N_H = number of neurons in the hidden layer
N_u = number of unknowns
p_j = excitation to neuron, j, $j = 1,2,\ldots,N_H$
Q = cost of function
r = random number in the range $[-1,1]$
s_k = excitation to neuron, k, $k = 1,2,\ldots,N_u$
t_k = estimates for the unknowns obtained with the ANN, $k = 1,2,\ldots,N_u$
x = spatial coordinate
x_l = entries of the neural network, $l = 1,2,\ldots,N$
Y = experimental (simulated) values for the radiation intensity
$\bar{Z}$ = vector of unknowns

Greek letters

β_i = total extinction coefficient, $i = 1 \ or\ 2$
$\Delta\bar{Z}$ = corrections of the unknowns
ε = tolerance for the iterative procedure sttoping criterion
$\eta^{(n)}$ = learning rates, $n = 1 \ or\ 2$
λ = damping parameter
μ = cosine of the polar angle
ρ_l = diffuse reflectivities, $l = 1,2,\ldots,4$
σ = standard deviation of measurement errors
σ_{s_i} = scattering coefficient, $i = 1 \ or\ 2$
ω = weights of the neural network connections

2. INTRODUCTION

The analysis of radiative transfer phenomena in multi-layer or heterogeneous participating media has attracted the attention of many researchers due to the relevant applications in different areas such as fire risk assessment [1], regional and global climate models [2], and Earth remote sensing [3], among several others.

In order to reduce the computation time for the solution of either the direct or inverse radiative transfer problems, artificial neural networks have been used [4-8].

Silva Neto and Soeiro [9] and Soeiro et al. [10, 11] have used Artificial Neural Networks (ANN) and hybrid methods for the estimation of radiative properties in one-dimensional homogeneous or heterogeneous participating media.

In the present work the formulation and solution of inverse radiative transfer problems with ANNs is presented for the estimation of the absorption and scattering coefficients in a two-layer media.

The patterns used in the neural network training were generated with the solution of the linear Boltzmann equation, which is used to model the direct radiative transfer problem.

A multi-layer perceptron neural network, with one hidden layer, is constructed for the solution of the inverse radiative transfer problem. In the input layer a total of N experimental data, with $N = 20$, is considered, and in the output layer there are four nodes, one for each unknown, i.e. the absorption and scattering coefficients of the two-layers.

As real experimental data was not available, we considered synthetic (simulated) data on the emerging radiation intensity with polar angle dependence, which was generated by adding a computationally generated pseudo-random noise to the calculated values obtained with the direct problem solution using the exact values of the parameters which are considered unknown in the inverse problem.

First only external detectors were considered, but the problem solution seems to be non-unique. Internal detectors were then also taken into account and the Artificial Neural Networks yielded good solutions for the inverse radiative transfer problem.

Refractive index effects [12] are not taken into account in the present work.

3. MATHEMATICAL FORMULATION AND SOLUTION OF THE DIRECT PROBLEM

Consider the problem of radiative transfer in a composite medium with two plane-parallel, isotropically scattering, gray layers, with diffusely reflecting boundary surfaces and interface, as shown in Fig. 1. The medium is subjected to external irradiation on both sides with intensity $f_1(\mu)$ at $x = 0$ and $f_2(\mu)$ at $x = L_1 + L_2$, where μ is the cosine of the polar angle, and L_1 and L_2 represent the thickness of layers 1 and 2, respectively.

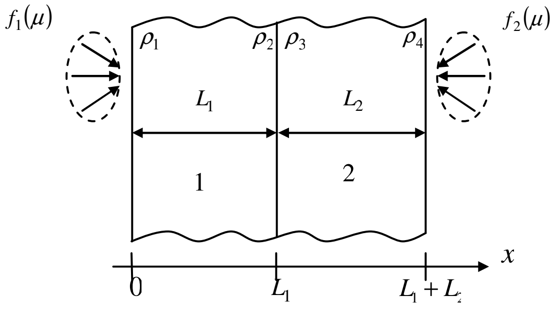

Fig. 1. Two-layer semitransparent medium.

The mathematical formulation of the direct steady-state radiative transfer problem with azymuthal symmetry is given by

Region 1

$$\mu \frac{\partial I_1(x,\mu)}{\partial x} + \beta_1 I_1(x,\mu) = \frac{\sigma_{s_1}}{2} \int_{-1}^{1} I_1(x,\mu')d\mu' \quad \text{in } 0 < x < L_1,\ -1 \le \mu \le 1 \tag{1a}$$

$$I_1(0,\mu) = f_1(\mu) + 2\rho_1 \int_0^1 I_1(0,-\mu')\mu' d\mu',\ \mu > 0 \tag{1b}$$

$$I_1(L_1,\mu) = (1-\rho_3) I_2(L_1,\mu) + 2\rho_2 \int_0^1 I_1(L_1,\mu')\mu' d\mu',\ \mu < 0 \tag{1c}$$

Region 2

$$\mu \frac{\partial I_2(x,\mu)}{\partial x} + \beta_2 I_2(x,\mu) = \frac{\sigma_{s_2}}{2} \int_{-1}^{1} I_2(x,\mu')d\mu' \quad \text{in } L_1 < x < L_1 + L_2,\ -1 \le \mu \le 1 \tag{2a}$$

$$I_2(L_1,\mu) = (1-\rho_2) I_1(L_1,\mu) + 2\rho_3 \int_0^1 I_2(L_1,-\mu')\mu' d\mu',\ \mu > 0 \tag{2b}$$

$$I_2(L_1 + L_2,\mu) = f_2(\mu) + 2\rho_4 \int_0^1 I_2(L_1 + L_2,\mu')\mu' d\mu',\ \mu < 0 \tag{2c}$$

where $I_i(x,\mu)$ represents the radiation intensity in layer i, with $i = 1 \, or \, 2$, β_i, is the total extinction coefficient

$$\beta_i = k_{a_i} + \sigma_{s_i} \tag{3}$$

k_{a_i} is the absorption coefficient, σ_{s_i} is the scattering coefficient and ρ_j are the diffuse reflectivities, with $j = 1, \ldots, 4$.

When the geometry, the radiative properties, and the boundary conditions are known, problem (1-2) may be solved yielding the values of the radiation intensities $I_1(x,\mu)$, for $0 \le x \le L_1$ and $-1 \le \mu \le 1$, and $I_2(x,\mu)$, for $L_1 \le x \le L_1 + L_2$ and $-1 \le \mu \le 1$. This is the direct problem.

For the solution of the direct problem we use in the present work a combination of Chandrasekhar's discrete ordinates method [13] with the finite difference method [14].

4. MATHEMATICAL FORMULATION AND SOLUTION OF THE INVERSE PROBLEM WITH ARTIFICIAL NEURAL NETWORKS (ANN)

We are interested in obtaining estimates for the vector of unknowns

$$\vec{Z} = \{\sigma_{s_1}, k_{a_1}, \sigma_{s_2}, k_{a_2}\} \quad (4)$$

using measured data on the emerging radiation intensity acquired at $x = 0$ and $x = L_1 + L_2$, Y_i, with $i = 1,2,\ldots,N$, being N the total number of experimental data.

As real experimental data was not available, we generated sets of synthetic experimental data with

$$Y_i = I_{\exp_i} = I_{calc_i}\left(\vec{Z}_{exact}\right) + \sigma r_i \quad (5)$$

where I_{calc_i} represents the calculated values of the radiation intensity using the exact values of the radiative properties, $\vec{Z}_{exact}$, which in a real application is not available and we want to determine with the inverse problem solution, σ simulates the standard deviation of the measurement errors, and r_i is a pseudo-random number generated in the range [-1, 1].

In order to solve the inverse radiative transfer problem we use here a multi-layer perceptron (MLP) neural network [15,16]. In Fig. 2 is given a representation of the MLP with the input and output layers, and one hidden layer for the solution of the inverse radiative transfer problem of determining the vector of unknowns $\vec{Z}$, given by Eq. (4), from the knowledge of the radiation intensities, Y_i, $i = 1,2,...,N$. By providing $\vec{Y}$ at the input layer we expect that the ANN will provide at the output layer an estimate for $\vec{Z}$.

Each neuron j, with $j = 1,2,\ldots,N_H$, in the hidden layer performs a linear combination of the input values provided at the input layer

$$p_j = \sum_{i=1}^{N} w_{ji}^{(1)} x_i + w_{j0}^{(1)} = \sum_{i=1}^{N} w_{ji}^{(1)} Y_i + w_{j0}^{(1)}, \quad j = 1,2,\ldots,N_H \quad (6)$$

where $w_{ji}^{(1)}$, $j = 1,2,...,N_H$, $i = 1,2,...,N$ are the weights of the connections between the nodes of the input layer and the neurons of the hidden layer, N is the number of nodes in the input layer, and N_H is the number of neurons in the hidden layer.

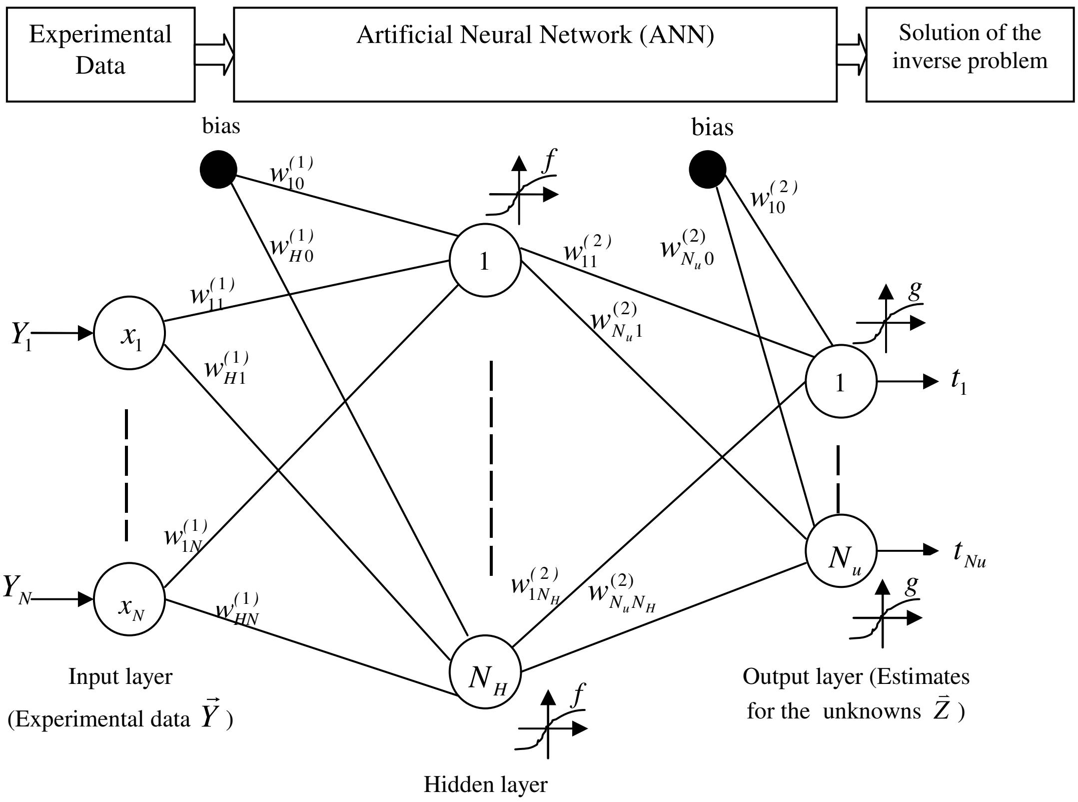

Figure 2 – Multi-layer perceptron network with one hidden layer for the inverse radiative transfer problem.

The weighted sum p_j given by Eq. (6) is viewed as an excitation to neuron j of the hidden layer, which provides in response

$$q_j = f(p_j), \quad j = 1,2,...,N_H \qquad (7)$$

where $f(.)$ is an activation function. Various choices for the function $f(.)$ are possible.

Each neuron k, $k = 1,2,...,N_u$ of the output layer performs a linear combination of the response q_j, $j = 1,2,...,N_H$, of the neurons of the hidden layer

$$s_k = \sum_{j=1}^{N_H} w_{kj}^{(2)} q_j + w_{k0}^{(2)}, \qquad k = 1,2,...,N_u \qquad (8)$$

where $w_{kj}^{(2)}$, $k = 1,2,...,N_u$, $j = 1,2,...,N_H$, are the weights of the connections between the neurons of the hidden layer and the neurons of the output layer, and N_u is the number of neurons in the output layer, which coincides with the number of unknowns of the inverse problem. Here we have $N_u = 4$ (see Eq. (4)).

The weighted sum s_k given by Eq. (8) is viewed as an excitation to neuron k of the output layer, which provides in response

$$t_k = g(s_k), \qquad k = 1,2,...,N_u \qquad (9)$$

where $g(.)$ is an activation function. Various choices for the function $g(.)$ are possible.

Combining Eqs. (6-9) we get

$$t_k = g\left(\sum_{j=1}^{N_H} w_{kj}^{(2)} f\left(\sum_{i=1}^{N} w_{ji}^{(1)} Y_i + w_{j0}^{(1)} \right) + w_{k0}^{(2)} \right)$$
$$k = 1,2,...,N_u \qquad (10)$$

Considering available the experimental data Y_i, $i = 1,2,...,N$, we observe in Eq. (10) that t_k, $k = 1,2,...,N_u$, are estimates for the unknowns Z_k, $k = 1,2,...,N_u$, obtained by the ANN. But before we can use Eq. (10) we must determine the weight parameters $w^{(1)}$ and $w^{(2)}$.

The determination of the weights $w^{(1)}$ and $w^{(2)}$ is accomplished by presenting a set of patterns (known input $\vec{Y}_{exact}$ and outputs $\vec{Z}_{exact}$) and calculating the weights that provides the best match between the calculated values $\vec{t}$ and the target values $\vec{Z}_{exact}$. The patterns used in this supervised training stage of the ANN were generated by calculating the values $\vec{Y}_{exact}$ from known sets $\vec{Z}_{exact}$ with the discrete ordinates and finite difference solution mentioned in the previous section.

For the determination of $w^{(1)}$ and $w^{(2)}$ we used the back propagation algorithm. We start with an initial guess for the weights, $w^{(1)n}$, $w^{(2)n}$, with $n = 0$, and the set of inputs $\vec{Y}$ is passed forward through the network yielding trial outputs $\vec{t}^{\,n=0}$ which are compared with the desired outputs $\vec{Z}_{exact}$ leading to the errors,

$$e_k^n = Z_{k exact} - t_k^n, \quad k = 1,2,...,N_u \qquad (11)$$

The weights are then adjusted using the information provided by the output error [15]

$$w_{kj}^{(2)n+1} = w_{kj}^{(2)n} + \eta^{(2)} \delta_k^{(2)n} q_j^n \qquad (11a)$$

$$w_{ji}^{(1)n+1} = w_{ji}^{(1)n} + \eta^{(1)} \delta_j^{(1)n} Y_i \qquad (11b)$$

where

$$\delta_k^{(2)n} = e_k^n g'(s_k^n) \qquad (12a)$$

$$\delta_j^{(1)n} = f'(p_j^n) \sum_{k=1}^{N_u} \delta_k^{(2)n} w_{kj}^{(2)n} \qquad (12b)$$

$\eta^{(1)}$ and $\eta^{(2)}$ are the learning rates, which can assume different values for the weights between input-hidden layers $^{(1)}$ and hidden-output layers $^{(2)}$.

The forward and backward sweeps procedure is continued until a convergence criterion related to errors e_k, $k = 1,2,...,N_u$, is satisfied.

The presentation of a full set of patterns is denominated epoch. After one epoch is completed the set of patterns is presented again, in a different (random) order. After a number of epochs, once the comparison error is reduced to an acceptable level over the whole training set, the training phase ends and the ANN is established. Therefore, in our inverse radiative transfer problem the unknowns $\vec{Z}$ (output) can be determined using the experimental data $\vec{Y}$ as the inputs to the ANN (see Fig. 2) and the simple forward sweep described by Eq. (10).

5. MATHEMATICAL FORMULATION AND SOLUTION OF THE INVERSE PROBLEM WITH THE LEVENBERG-MARQUARDT METHOD (LM)

As the number of experimental data available is larger than the number of unknown parameters to be determined, the inverse problem may be formulated implicitly as an optimization problem, in which we seek to minimize the squared residues cost function

$$Q\vec{Z} = \sum_{i=1}^{N} \left[I_{calc_i}\left(\vec{Z}\right) - Y_i \right]^2 = \vec{F}^T \vec{F} \qquad (13)$$

where the elements of the vector of residues given by

$$F_i = I_{calc_i}\left(\vec{Z}\right) - Y_i, \quad i = 1,2,\ldots,N \qquad (14)$$

From the critical point equation

$$\frac{\partial Q\left(\vec{Z}\right)}{\partial \vec{Z}} = 0 \qquad (15)$$

one obtains the system of non-linear equations

$$J^T \vec{F} = 0 \qquad (16)$$

where the elements of the Jacobian matrix are given by

$$J_{ij} = \frac{\partial I_{calc_i}}{\partial Z_j}, \quad i = 1,2,\ldots,N \quad and \quad j = 1,2,\ldots,N_u \qquad (17)$$

Writing a Taylor's expansion and keeping only the terms up to the first order

$$\vec{F}\left(\vec{Z}^{n+1}\right) = \vec{F}\left(\vec{Z}^{n}\right) + J^n \Delta\vec{Z}^n \qquad (18)$$

where

$$\vec{Z}^{n+1} = \vec{Z}^n + \Delta\vec{Z}^n \qquad (19)$$

and introducing Eq. (18) in Eq. (16) results

$$J^{T^n} J^n \Delta\vec{Z}^n = -J^{T^n} \vec{F}^n \qquad (20)$$

Adding a damping factor λ^n to the diagonal terms of the matrix $J^T J$ one gets the well known Levenberg-Marquardt method

$$\left(J^{T^n} J^n + \lambda^n \Im \right) \Delta\vec{Z}^n = -J^{T^n} \vec{F}^n \qquad (21)$$

where $\Im$ represents the identity matrix.

An iterative procedure is then constructed by starting with an initial guess $\vec{Z}^0$ and then calculating $\Delta\vec{Z}^n$ and $\vec{Z}^{n+1}$ with Eqs. (21) and (19) respectively, with $n = 0,1,2,\ldots$ until a prescribed stopping criterion is satisfied, such as

$$\left| \frac{\Delta Z_i^n}{Z_i^n} \right| < \varepsilon \qquad (22)$$

where ε represents a small tolerance, say 10^{-5}.

6. RESULTS AND DISCUSSION

In Table 1 we present the results obtained with the LM method starting with the initial guess: $\sigma_{s_1} = 0.10\ cm^{-1}$, $k_{a_1} = 0.8\ cm^{-1}$, $\sigma_{s_2} = 0.10\ cm^{-1}$ and $k_{a_2} = 0.8\ cm^{-1}$ for the particular case with the exact values for the unknowns $\sigma_{s_1} = 0.45\ cm^{-1}$, $k_{a_1} = 0.05\ cm^{-1}$, $\sigma_{s_2} = 0.45\ cm^{-1}$ and $k_{a_2} = 0.05\ cm^{-1}$ (maximum noise in the experimental data = 8% - σ = 0.002 in Eq. (5)) . Note that these LM does not converge with these estimates after 10 iterations.

For the test case presented it is also considered $L_1 = L_2 = 2cm$, $\rho_1 = 0.1$, $\rho_2 = \rho_3 = 0$, $\rho_4 = 0.9$, $f_1 = 1.0$ and $f_2 = 0$, which represents a difficult test case.

Table 1 – Estimates obtained with LM (10 iterations). Noisy data (8%)

Iteration	σ_{s_1} cm^{-1}	k_{a_1} cm^{-1}	σ_{s_2} cm^{-1}	k_{a_2} cm^{-1}	*Obj. Func. [Eq.(13)]*
0	0.10	0.8	0.10	0.8	7.439
5	0.52	0.049	2.1E09	0.01	6.86E-01
10	0.45	0.05	5.5E07	3.7E07	1.216

In Table 2 are shown the results for the same test case using ANNs, and in Tables 3 and 4 are presented the results obtained when the ANN is used to generate the initial guess for the LM method. Here we used noisy data (maximum 8%), i.e., σ = 0.002 in Eq. (5). The experimental data used for the solution of the inverse problem consisted of a set of 40 radiation intensities measured at different polar angles, 20 intensities measured by external detectors and 20 intensities measured by internal detectors located at the interface between the two-layers, i.e. $x = L_1$.

Therefore, there are $N = 40$ entries in the input layer of the ANN. For the hidden layer we considered $N_H = N = 40$. We used 500 patterns (N_P) and a decreasing number of epochs (N_E) in order to save computational time.

In this work the Neural Network Toolbox of the software MATLAB (Mathworks, Inc.) was used with the following neuron model in the backpropagation network: 40 elements in the input vector, log-sigmoid (logsig) transfer function between the input layer and the hidden layer (with 40 elements) and a linear transfer function (purelin) in the output layer (with 4 elements in the output vector).

Table 2 – Neural Network solutions for the inverse problem and CPU time considering different number of epochs ($N_H = 40$, $N_P = 500$) and noisy data (8%)

N_E	*CPU time(min)*	Estimates (ANN)			
		σ_{s_1} cm^{-1}	k_{a_1} cm^{-1}	σ_{s_2} cm^{-1}	k_{a_2} cm^{-1}
500	120	0.40	0.01	0.43	0.01
200	48	0.34	0.01	0.33	0.01
100	22	0.35	0.09	0.32	0.09
30	7,5	0.50	0.10	0.60	0.05

It can be observed from Table 2 that the ANN did not provide good estimates for the unknowns. An improvement can be obtained, but at the expense of a higher CPU time requirement. A different strategy is then adopted with a hybridization ANN-LM.

In Table 3 are presented the results obtained with a hybridization ANN-LM in which the former method provides an initial guess for the latter. The solution of the ANN were obtained considering 100 epochs in the training stage of the ANN. Now the results of the inverse problem are much better.

Table 3 - Using ANN to obtain estimates for the LM with noisy data and number of epochs $N_E = 100$

Noise	ANN estimates				Results (LM)			
	σ_{s_1} cm^{-1}	k_{a_1} cm^{-1}	σ_{s_2} cm^{-1}	k_{a_2} cm^{-1}	σ_{s_1} cm^{-1}	k_{a_1} cm^{-1}	σ_{s_2} cm^{-1}	k_{a_2} cm^{-1}
8%	0.35	0.09	0.32	0.09	0.447	0.050	0.455	0.050
4%	0.40	0.03	0.45	0.04	0.450	0.050	0.445	0.049
2%	0.39	0.04	0.42	0.05	0.450	0.049	0.449	0.050
0%	0.37	0.04	0.40	0.05	0.45	0.05	0.45	0.05

In Table 4 are shown the results obtained using also the hybridization ANN-LM, but now with only 30 epochs in the training stage of the ANN. It can also be observed that very good results are obtained for the inverse problem.

Table 4 - Using ANN to obtain estimates for the LM with noisy data and number of epochs $N_E = 30$

Noise	ANN estimates				Results (LM)			
	σ_{s_1} cm^{-1}	k_{a_1} cm^{-1}	σ_{s_2} cm^{-1}	k_{a_2} cm^{-1}	σ_{s_1} cm^{-1}	k_{a_1} cm^{-1}	σ_{s_2} cm^{-1}	k_{a_2} cm^{-1}
8%	0.50	0.10	0.60	0.05	0.447	0.050	0.455	0.050
4%	0.49	0.01	0.47	0.01	0.450	0.050	0.445	0.049
2%	0.54	0.03	0.53	0.04	0.449	0.050	0.449	0.050
0%	0.51	0.02	0.49	0.04	0.45	0.05	0.05	0.45

It must be stressed that the solution of the inverse problem with either the LM or ANN methods using only external detectors led to non-unique solutions of the inverse radiative transfer problem.

7. CONCLUSIONS

A hybridization ANN-LM was successfully implemented for the estimation of the absorption and scattering coefficients in two-layer participating media even in the presence of noisy data. A test case demonstrates that the ANN may provide good initial estimates for the LM.

Internal detectors, which were located at the interface between the two layers, were necessary in order to yield unique solutions for the inverse problem.

ACKNOWLEDGEMENTS

The authors acknowledge the financial support provided by CNPq – Conselho Nacional de Desenvolvimento Científico e Tecnológico – and FAPERJ – Fundação Carlos Chagas Filho de Amparo à Pesquisa do Estado do Rio de Janeiro.

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