Retrieval of particle parameters with the neural network using multi-angle light-scattering data

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A method to retrieve radius and refractive index of spherical homogeneous non-absorbing particles by multi-angle scattering is proposed. It is based on formation of the noise resistant functionals of intensity, which are invariant relative to linear homogeneous transformations of an intensity-based signal, and approximation of the retrieved parameters' dependence on the functionals by a feed-forward neural network. The method allows reducing retrieval errors in the region of small sizes and refractive indices of particles close to unity.

INTRODUCTION

The problem of retrieval of disperse particle characteristics often arises in science and engineering. Efforts of researchers to solve this problem have led to the evolution of numerous methods. The choice of the method depends on particle characteristics and measurement conditions. Among the choices are light-scattering methods that are fast and noninvasive [1].

The problem of particle parameter retrieval belongs to one type of inverse problems. In recent years, the neural-network method is widely used to solve the inverse light scattering problems [2, 3]. In the neural-network method, the main computer time is spent in training the network. Once trained, the network determines the particle characteristics very quickly. Large stability to random errors can be achieved. These are the advantages of the method. In the present paper, the feed-forward neural network is used to retrieve parameters of homogeneous spherical particles using multi-angle scattering data.

CONSTRUCTION AND TRAINING OF A NEURAL NETWORK

We consider a problem of retrieval of a particle radius R and relative refractive index n by the intensity of light scattered in the interval of angles from 10° up to 60°. This range of angles is available for measurements in a new generation of scanning flow cytometers [4]. The particle is illuminated by a non-polarized beam of light. The wavelength λ of the incident light in a medium is equal to 0.476 μm. The particle radius ranges from 0.6 μm to 13.6 μm, the relative refractive index ranges from 1.015 to 1.28. To retrieve the particle parameters the feed-forward neural network is used [5].

An element of the neural network is a neuron, which calculates the weighted sum of signals entered as its input and transforms the results according to a non-linear function.

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Using the redistribution system, the signals from the outputs of neurons of the first layer are passed to inputs of the neurons of the second layer. The neurons of the second layer process the signal in the same manner as the first one and pass the signal to the input of the neuron of the next layer. The output signal of the *N*-layer neuron network of forward propagation is:

$$y_l^{out} = F\left(\sum_k w_{lk}^N y_k^N = \cdots F\left(\sum_j w_{tj}^2 y_j^2 = F\left(\sum_i w_{ji}^1 y_i^1 = y_i^{in}\right)\right)\right). \tag{1}$$

Here y_i^1, y_j^2, … , y_k^N are the signals at inputs of the 1st, 2nd , …, *N*th layer of the neural network, w_{ji}^1, w_{ji}^2,…, w_{lk}^N are the weight coefficients of the neurons of the 1st, 2nd , …, *N*th layer of the neural network; *F*(x) is the neuron activation function [5].

Usually, vectors of input signals for each layer contain the permanent unit signal y_0^n, where n = 1, 2, 3. It is supposed that all neurons have an identical activation function. We use the continuous function which is obtained from the function given in [6]:

$$F(x) = \frac{1}{x_{\max} - x_{\min}}\left(\sqrt{\beta + (x - x_{\min})^2} - \sqrt{\beta + (x - x_{\max})^2}\right), \tag{2}$$

where $x_{\min}$, $x_{\max}$, and β are parameters.

Simplicity and an opportunity to change the form of the activation function in a wide range are advantages of Eq. (2). We used the function $F(x)$ at $x_{\min}$ = -1, $x_{\max}$ =1, and β = 0.1. From Eq. (2), it is easy to obtain an expression for derivative of function $F(x)$, which is used at the neural-network training:

$$F'(x) = \frac{1}{x_{\max} - x_{\min}}\left(\frac{x - x_{\min}}{\sqrt{\beta + (x - x_{\min})^2}} - \frac{x - x_{\max}}{\sqrt{\beta + (x - x_{\max})^2}}\right). \tag{3}$$

To train the neural network, it is necessary to find weight coefficients of the neurons of all layers using the least-squares minimization method. It is better to minimize relative errors of measurements than the absolute ones, as the particle parameters can vary in a wide range. It leads to a problem of the minimization of a square-law form at training of the neural network for determination of radius

$$\Phi = \frac{1}{2}\sum_{\alpha=1}^{N_B}\left(\frac{y^{out}\left(w_{ji}^1,\ldots,w_k^N, y_{i\alpha}^{in}\right)}{R_\alpha} - 1\right)^2 \tag{4}$$

and relative refractive index

$$\Phi = \frac{1}{2}\sum_{\alpha=1}^{N_B}\left(\frac{y^{out}\left(w_{ji}^1,\ldots,w_k^N,y_{i\alpha}^{in}\right)-1}{n_\alpha-1}-1\right)^2, \tag{5}$$

respectively. Here α = 1, 2, …, N_B, and N_B is the number of samples in the training database.

After transformations of Eqs. (4) and (5), we can write

$$\Phi = \frac{1}{2}\sum_{\alpha=1}^{N_B}\frac{1}{s_\alpha^2}\left(y^{out}\left(w_j^1,\ldots,w_{lk}^N,y_{i\alpha}^{in}\right)-p_{n\alpha}\right)^2. \tag{6}$$

Here $p_{n\alpha}$ is the normalized value of parameter $\sigma_\alpha = R_\alpha - a_R$ in training of the neural network at the radius determination and parameter $s_\alpha = n_\alpha - a_n - b_n$ in training of the neural network at the relative-refractive-index determination. To solve the optimization problem Eq. (6), the limited memory BFGS method [7] was used.

Calculations show that the criterion function $\Phi\left(w_{ji}^1,\ldots,w_{lk}^N,y_{i\alpha}^{in}\right)$ has many minima, where values are approximately the same. In such conditions, searching of a global minimum can take vast amounts of time. Therefore, we found three (or four) local minima, starting from the point with coordinates chosen by the random-number generator from the interval [-1, 1]. We used the minimum providing the minimal value of the criterion function.

ESTIMATION OF ERRORS OF PARTICLE PARAMETERS RETRIEVAL

In training the neural network, we used the book of problems containing 10^4 samples randomly chosen from the range of considered parameters. If the set of samples is insufficiently representative, the stability of the neural network to input data changes is low. The neural network well trained on the samples from the book of problems can give significant errors on the other samples. We verified the work of the neural network using 10^4 samples which were different from the samples used in the neural-network training. To increase the stability of the neural network, the amount of the neurons of the internal network layers was decreased and random noise in the input data was introduced.

The correlation dependences of the original values of parameters R and n and the retrieved values of R_e and n_e were obtained. The values of R_e and n_e were calculated using the three-layer neural network with 10 neurons in the internal layer. Comparison with the results obtained with the neural networks trained with the minimal absolute error revealed that the proposed technique enables the parameter retrieval error in the interval of small sizes and close to unity relative refractive indices to be essentially reduced.

The mean relative error of radius retrieval was estimated as follows:

$$\delta R = \frac{1}{A}\sum_{\alpha=1}^{A}\left|1-\frac{R_{e\alpha}}{R_\alpha}\right|, \tag{7}$$

where $R_{e\alpha}$ are the retrieved values of radius; R_α is the original value of radius.

To evaluate the error of the relative refractive index retrieval the quantity was used

$$\delta n = \frac{1}{A}\sum_{\alpha=1}^{A}\left|1-\frac{n_{e\alpha}-1}{n_\alpha-1}\right|. \tag{8}$$

Here $n_{e\alpha}$ are the retrieved values of relative refractive index; n_α is the original value of relative refractive index.

CONCLUSION

A method to retrieve radius and relative refractive index of non-absorbing homogeneous spherical particles by light scattered in the range of angles 10^o – 60^o is proposed. It is based on the construction of the scattered intensity signal, which is invariant with respect to the linear homogeneous transformations, and on the approximation of the dependence of the retrieved parameters on the signal functionals by the neural network of forward propagation.

To verify the proposed technique, experimental data [4] on angular dependences of scattered light obtained by the scanning flow cytometry were used. We retrieved the particle parameters by the neural network and by the least-squares method. The relative deviation of parameters found with the neural network and the least-squares method does not exceed 4.3 % for radii and 3.8 % for refractive index.

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