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Novel approaches to structural reconstruction of scattering media using machine learning

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The work is devoted to advancing the idea of using machine learning technology combined with the algorithmic Monte Carlo method to reconstruct the spatial location of scattering centers in the corneal tissue, as well as the density distribution of these centers within the volume during longitudinal scanning of the sample. A favorable prediction is observed for reproducing the sample thickness along with determining the location of each scattering center. The Monte Carlo generated “heat map” of the probability of photon exit coordinates from the investigated medium is used as a set of input data for training the neural network. The proposed convolutional neural network architecture made it possible to achieve up to 98% accuracy in reconstructing the spatial location of scattering centers and the density distribution of these centers during longitudinal scanning.

Keywords: Neural network, machine learning, Monte Carlo, amplitude (phase) function, OCT.

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Introduction

Optical coherence tomography (OCT) is a non-contact method for visualizing the structure of a medium that enables high-resolution imaging of transverse and longitudinal tissue sections [1-3]. In particular, OCT methods are used to study transparent (semi-transparent) objects, such as the cornea of the eye [2].

A special place in the development of OCT methods is occupied by polarization-sensitive (PS) [4] research methods that allow studying the change in the polarization state of the beam during its interaction with a polarization-active object. By analyzing corresponding variations in the interference channels of the two arms of a Mach-Zehnder interferometer, it becomes possible to reconstruct the structure of thin corneal nanolayers even at scanning depths smaller than the longitudinal coherence length. In the context of the proposed approaches, we previously demonstrated [5-7], the unique opportunity to non-

invasively obtain information about the structure of thin layers of transparent objects even when they are destroyed or damaged. Our most recent studies [8-10] are aimed at further developing the method of polarization-sensitive optical coherence tomography, by introducing the concepts of geometric and dynamic phase [8-10] and using a modified Mach-Zehnder interferometer configuration [5-10]. In these works, within the framework of the developed polarization Monte Carlo model, we evaluated the depolarization of the signal and proposed methods to increase the accuracy of structural reconstruction by 22% [9,10].

At the same time, to construct a complete tomographic image within the framework of PS methods, it is necessary to determine the spatial location of the scattering centers, their density and their depth distribution when scanning into the sample, which at the stage of the previously presented studies was an open question.

Currently, there are studies [11,12], that involved a combination of the Monte Carlo method with the use of neural networks to reproduce the spatial properties of the scattering medium. However, these approaches require an additional estimation of the scattered-radiation intensity for different distances (thicknesses) of the medium, using either information about the backscattered intensity profile (the dependence of backscattered intensity on the distance between the receiver and the source) [11], or the angular distribution of the intensity [12].

In this work, we propose an original solution based on the use of probabilistic photon-exit coordinate data obtained via the Monte Carlo method, without taking photon energy into account, to construct a “heat map”, that is combined with our custom machine-learning algorithm. This approach makes it possible to reconstruct the three-dimensional arrangement of scattering centers with an accuracy of about 97%. Thus, the current problem of reproducing the coordinates of the centers throughout the depth of the longitudinal scan is solved. This approach can be applied to the study of the spatial structure of transparent/semitransparent media not only in back-reflected/backscattered radiation but also in forward-transmitted radiation.

I. Formation of a comparative database for training and testing the neural network in combination with the Monte Carlo method

The scattering centers of the cornea, which are the objects of investigation in this work, as epithelial cell nuclei of the epithelium and keratocytes located between the stromal lamellae [5], define the scattering of the incident photon packet. In Monte Carlo approaches [13,14], this scattering is described by the amplitude and phase scattering functions. The particles are optically soft, the condition $|m-1| \ll 1$ is satisfied, where m is their relative refractive index, the scattering of light on which described using of the Van de Hulst approximation or the “anomalous diffraction” theory [15-20].

In the approximation of this method, a set of random numbers is used to model stochastic processes that define the probabilistic nature of photon scattering on the scattering centers. In tasks of photon transport description this approach is implemented by simulating a large number of individual photon trajectories that pass through the medium in a random manner, undergoing scattering, absorption, or reflection. The nature of each interaction is given by statistical parameters of the medium - such as the scattering coefficient (μ_s), the absorption coefficient (μ_a), the attenuation coefficient ($\mu = \mu_s + \mu_a$), and the anisotropy parameter (g), which determines the probable direction of photon deflection after scattering.

As a rule, the Monte Carlo model [5–10] involves estimating parameters such as the photon free path length $l = -\frac{\ln \xi}{\mu}$ to the next interaction event (ξ is a random variable uniformly distributed in the interval $[0; 1]$), as well as the azimuthal (φ) and polar (θ) scattering angles, which are sampled according to the distribution of the

phase function $P(\theta, \varphi)$ interpreted as a probability density function. Another parameter is the weight of photon packets after the i -th scattering event: $W_i = P(\theta_i, \varphi_i) \cdot W_{i-1}$. When scattering occurs at angles θ, φ , the photon packet weight decreases according to the value of the phase function $P(\theta, \varphi)$; i is the index of the scattering event. The mean number of scattering events N_s is proportional to the ratio z/l_s [5], $l_s = 1/\mu_s$ is the scattering length (the mean distance between scattering centers). Among the scattering parameters chosen for evaluation, and used by us to form the comparison database for neural network training, are the scattering coefficient and the scattering length. The maximum possible concentration of scattering centers is limited by particle size $\rho_N^{max} = 1/V_0$, where V_0 is the particle volume (for spherical particles, $V_0 = \frac{4}{3}\pi a^3$, here a is a particle radius). Simulation of the interaction of the photon packet with the scattering medium was carried out with the phase function, within the approximation of van de Hulst’s anomalous diffraction theory.

As input parameters, we select the initial weight of photon packets $W = 1$, the number of packets 10^5 , and the initial position of the photon in the x-y plane is subject to the Gaussian law, with a half-width $w_0 \approx 15 \mu\text{m}$. The average initial beam intensity is $I_0 = \frac{1}{N} \sum_{i=1}^N W_i = 1$, where N is the number of photons in a photon packet (in the first approximation we set $N = 1000$). We assume that the initial weight of all photon packets is uniform across the entire transverse cross-section, and we take the wavefront to be flat. Then the probability density function of the photon distribution can then be written as

$$p(x, y) = \frac{e^{-\frac{x^2+y^2}{2w_0^2}}}{2\pi w_0^2},$$

which is directly related to the probability of photon exit coordinates. The statistical parameters of the photon distribution change depending on the medium thickness (z), the particle size (a or $\chi = ka$, where $k = \frac{2\pi}{\lambda}$ is a wave number, λ – wavelength in vacuum), and the scattering coefficient μ_s .

The resulting probability distribution of photon exit coordinates in the form of a “heat map,” i.e., a thermal color distribution, is shown in Fig. 1. The values of the obtained coordinates, normalized by the value w_0 , are plotted along the x, y axes, which allowed us to present the “heat map” without being tied to the absolute transverse dimensions of the beam. The color scale corresponds to the local probability density $p(x, y)$. For the convolutional neural network (CNN) training, that is used as a neural network the coordinates on the “heat map” are normalized in the range from 0 to 1 (Fig.2). Such distributions (normalized “heat maps”) with different averaging steps ($\Delta x, \Delta y$), for different particle size parameters (χ) and at different z/l_s ratios are shown in Fig. 2. Reducing the averaging step produces more pronounced patterns of information reproduction about the coordinate distribution of photon output (Fig. 1,2 (a,b)).

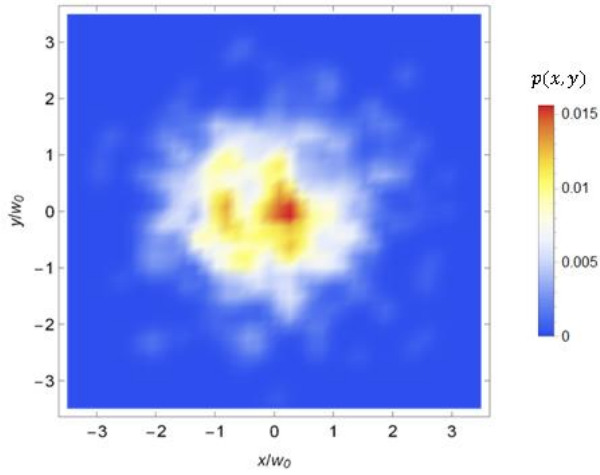


Fig.1. Probability histogram of the coordinate distribution of the output of 1000 photons. Averaging with a step $\Delta x, \Delta y = 0.14w_0$.

The change in the position of photons in space (trajectories) (Fig. 2c) corresponding to different “heat maps” (Fig. 2a, b) are obtained for different layer thicknesses d . In particular, Fig. 2 (a, b) presents a sample of two values of layer thicknesses (d) at the case of the

longitudinal scanning (z): $2l_s$ and $3l_s$ for a step $\Delta x, \Delta y = 0.06$ a.u. (normalized coordinates) and size parameter of particles $\chi = 24$.

The obtained photon trajectories allow us to make predictions about the location of the scattering centers, based on the conditional areas of change in the photon trajectory. Naturally, the change in the photon trajectory (highlighted with ovals in Fig. 2c) occurs within certain planes (Fig. 2d), which are located in the vicinity of the scattering centers, at distances multiples of l_s .

II. Neural network training

The obtained set of thousands “heat maps” are used by us to train the neural network, without using additional information about the energy changes of the photon flows at the exit from the studied medium. A convolutional neural network (CNN) was chosen as the working neural network, which allowed us to predict the key characteristics of the corneal tissue, based on the data obtained by the Monte Carlo method.

The constructed architecture of neural network allows one to analyze local distribution patterns, such as peaks in the photon probability density distribution, which may

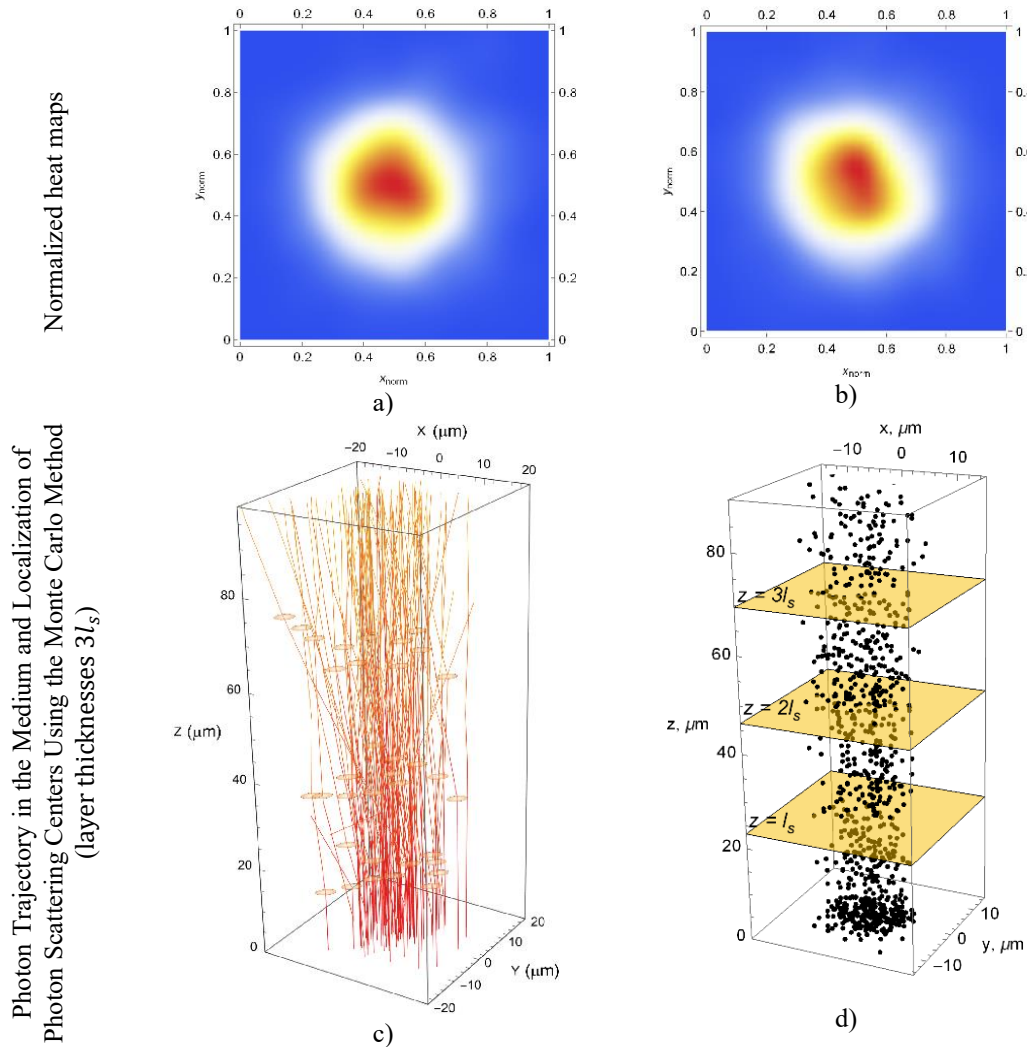


Fig. 2. Normalized “heat maps” for layer thicknesses $2l_s$ and $3l_s$ (a, b), photon trajectories within the medium (c) (ovals mark the change in the trajectory of photons), with reconstructed positions of the planes corresponding to the localization of scattering centers (d).

indicate the layer thickness and the distribution of scattering centers. The model is built on a balance between accuracy and computational efficiency, which made it possible to avoid overtraining and "dead neurons". In developing the algorithm, several key functions were implemented, such as a Dropout function, which prevents overtraining by randomly ignoring 40% of the connections formed at each stage of the training iteration, a standard ReLU activation function, which removes negative intensity values, and the Batch Normalization function, which stabilizes activation statistics, eliminating internal sliding bias between training iterations, contributes to faster convergence and increased model stability, ensuring signal averaging, reproducibility of small elements with significant acceleration of the neural network training process. The MaxPooling function acts as a filter that highlights regions with the highest photon exit probabilities, progressively refining and reducing the size of the analysis regions while preserving key local extrema that represent areas of maximum intensity.

During algorithm implementation, a "feature vector" was formed as a set of numbers representing the probability of light scattering through the depth of the studied layer and the probabilistic estimate of photon exit. The resulting feature vector corresponds to discretized zones of the photon distribution associated with the anisotropy of optical properties. This allowed the neural network to infer how light was scattered within the cornea.

The current neural network architecture model is based on a sequence of convolutional layers for image processing, followed by integration with environmental parameters and fully connected layers for regression. The network does not observe individual photons; however, during training, it predicts the structure of the medium. The model represents an optimized and developed version of previous approximations, which used either fewer filters (32-64) or alternative activation/regularization functions during hardware implementation of the machine learning process.

Overall, according to the neural network architecture, the convolutional layers analyze the «heat maps» to identify macroscopic patterns, such as regions of high photon concentration, which indicate probable values of tissue layer thickness and the location of scattering centers. The fully connected layers combine these probability distribution regions with environmental parameters (μ_s , g) to reconstruct the layer thickness (z), scattering coefficient (μ_s), and coordinates of scattering centers. The ReLU activation function introduces nonlinearity, enabling the model to capture complex relationships between the planar structure of the heat map and the physical properties of the tissue. Dropout (0.4) ensures robustness to variations in input data, noise in the heat maps, varying photon counts, or minor shifts. The total number of model parameters is $\sim 8 \times 10^5$, which is sufficient to accurately reproduce the optical properties of the cornea without excessive computational complexity. The use of `batch_size = 64` function allows simultaneous processing of 64 heat maps per step, significantly accelerating the training process. All photons exit probability values on the "heat maps" are represented in the range $[0, 1]$, where the darkest pixel = 0 and the brightest = 1.

The neural network was developed in Python using the TensorFlow library. The model was trained using the Adam optimizer (learning rate 10^{-3}) with the data distribution: 70% training, 20% validation, 10% test. To stop the model training, the EarlyStopping function was employed, which activated when the validation error increased, that is, when model accuracy ceased to improve and further iterations only added noise. Thus, the neural network was protected from overtraining while preserving the optimal model. During the neural network training process, the model's performance is evaluated at each training step using the loss function L , taking into account the relative error $\varepsilon(P_i)$ of the prediction

$$L = \sum_{i=1}^3 W_i \cdot \varepsilon(P_i).$$

Gradual improvement of the architecture and an increase in the number of photons in the packet (N) make it possible to reduce the probabilistic nature of the simulation, which results from using the Monte Carlo method. For example, increasing the number of photons in the photon packet also reduces the absolute error σ in reconstructing the positions of scattering centers and determining the thickness of the layer in which the centers are distributed, compared to the data used to train the neural network from 13% for 1000 photons to 2% for 5000 photons in the photon packet.

The result of the Monte Carlo simulations and the neural network training is the determination of the locations of the scattering centers for 5000 photons in the input photon packet, along with the estimation of the layer thickness z for different photon mean free paths, as shown in Fig. 3.

An interesting observation is that the neural network reconstructs the positions of the scattering centers not only in the XY plane, but also predicts their localization with respect to variations in the thickness of the studied layer, forming holistic three-dimensional picture of the location of scattering centers of the cornea.

As can be seen from the images above (Fig. 3), as the neural network is trained, the positions of the scattering centers are refined to achieve the maximum probability of determining their spatial position. The neural network is able to predict the three-dimensional distribution of scattering centers and the heterogeneity of their location. Moreover, the proposed architecture allows us to reproduce the characteristics of the layers regardless of the trajectory of photons inside the layer. Accordingly, the coordinates of the scattering centers help predict the position of structural scattering elements, structural deformation, and volumetric density of the location, which is compared with the OCT picture obtained for normalized (ideal) images of the existing coherence tomography database. Thus, training the neural network makes it possible to increase the accuracy of structure reconstruction up to 98%, practically reaching the level of complete repeatability of the results.

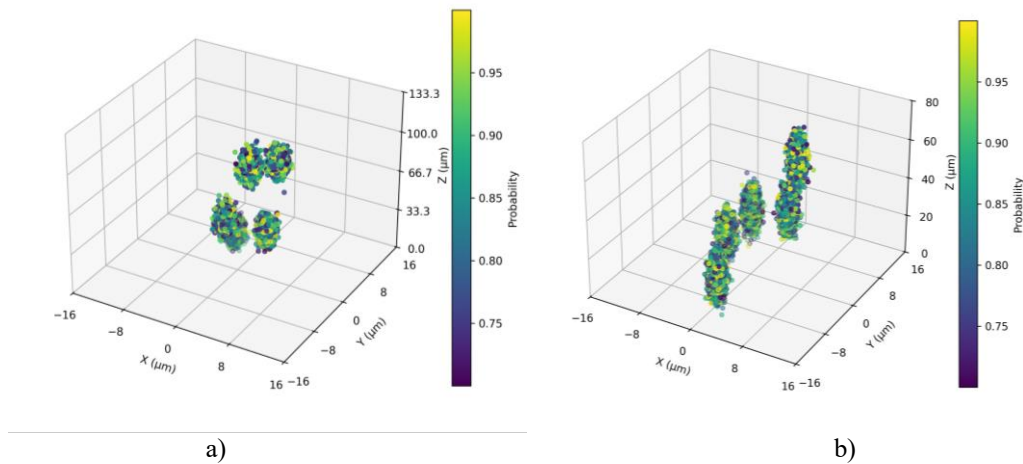


Fig. 3. Prediction of the locations of scattering centers for $N = 5000$ for different layer thicknesses: a) $1.2l_s$ b) $2l_s$.

Conclusions

This study develops an approach that integrates the algorithmic Monte Carlo method with the designed machine learning model to reconstruct the spatial distribution of scattering centers in the corneal tissue. The method also enables the evaluation of the volumetric density of these centers and the determination of sample thickness during longitudinal scanning.

The proposed Monte Carlo-based algorithm for generating a “heat map” provides probabilistic coordinates of photon exit points from the investigated medium, which are then used as the input dataset for training the neural network. The developed convolutional neural network demonstrates high accuracy up to 98% in reconstructing both the spatial arrangement and volumetric density of scattering centers during longitudinal scanning. Importantly, the model operates independently of the specific photon trajectories within the medium and does not require information about photon intensity or the beam’s intensity profile at the output of the sample. This makes the approach universal and promising for further integration into modern optical coherence tomography techniques.

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Нові розв'язки відтворення структури розсіювальних середовищ з використанням технології машинного навчання

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Робота присвячена розвитку ідеї використання технології машинного навчання, яка поєднується з алгоритмічним методом Монте-Карло, для відтворення просторового розташування розсіювальних центрів рогівки ока, щільності розподілення центрів в об'ємі при скануванні зразка у повздовжньому напрямку. Спостерігається сприятливий прогноз по відтворенню значення товщини зразка з визначенням місця розташування розсіювального центра. Отримана, методом Монте-Карло, «теплова карта» ймовірності координат виходу фотонів з досліджуваного середовища, використовується як набір входних даних для тренування нейронної мережі. Запропонована архітектура згорткової нейронної мережі дозволило досягнути точності відтворення просторового розміщення розсіювальних центрів, щільності розподілу центрів, при повздовжньому скануванні, до 98%.

Ключові слова: Нейромережа, машинне навчання, Монте-Карло, амплітудна (фазова) функція, ОКТ.