

# Materials Research Express



## PAPER

### OPEN ACCESS

#### RECEIVED

30 October 2019

#### REVISED

10 November 2019

#### ACCEPTED FOR PUBLICATION

4 December 2019

#### PUBLISHED

17 February 2020

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## Determination of material optical properties from diffusive reflection light intensity profiles at multiple distances

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**Keywords:** scattering coefficient, absorption coefficient, isotropic coefficient, refractive index, optical measurement, optical property, neural network

### Abstract

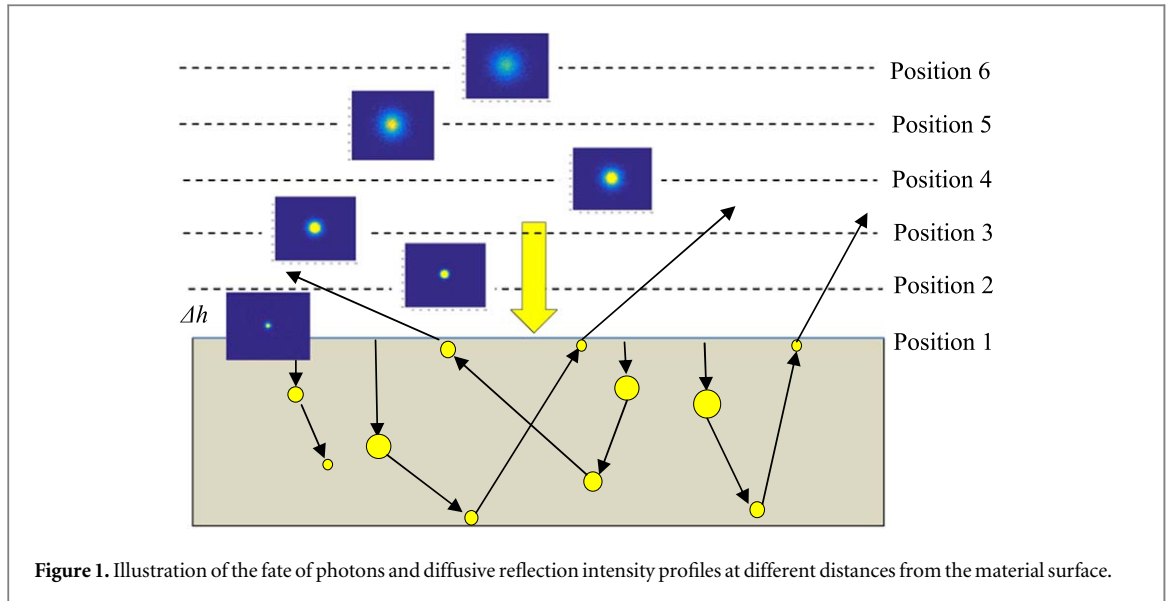
Optical absorption and scattering properties are often estimated from the diffusive reflection light intensity at only one distance from the material surface, which often encounters accuracy and convergence issues. In this work, a method was proposed to determine optical properties by using diffusive reflection light intensity profiles at multiple distances, which enhanced data richness as a result of the intensity profiles are linearly independent. In this method, five features of light intensity profiles (contrast, correlation, energy, homogeneity, and second moment) were used to reduce the data dimensions. To demonstrate the effectiveness of the proposed method, Monte Carlo (MC) simulations were used to generate diffusive reflection light intensity profiles with noise at different distances for various combinations of four optical properties (absorption coefficient  $\mu_a$ , scattering coefficient  $\mu_s$ , isotropic coefficient  $g$ , and refractive index  $n$ ). The five profile feature vectors were used as inputs and the four optical parameters were used as outputs to train and test a backpropagation (BP) neural network. The influences of noise levels and the number of diffusive light intensity profiles on parameter estimation accuracy were investigated. The four optical parameters estimated by the BP network were compared with the results estimated by the traditional least squares method, which shows that the proposed method can estimate the optical properties with higher accuracy and better convergence.

## 1. Introduction

Optical properties such as absorption coefficients ( $\mu_a$ ), scattering coefficients ( $\mu_s$ ), isotropic coefficients ( $g$ ), and refractive index ( $n$ ) are related with material chemical composition and physical properties [1]. They are very useful in medical diagnosis, food and agricultural product quality measurement, pollution detection, and many other applications [2, 3]. Hence, much attention has been paid to determine absorption coefficients  $\mu_a$  and reduced scattering coefficients  $\mu'_s = (1-g)\mu_s$  of materials over the past 30 years.

When photons propagate in a turbid media, it may be absorbed, scattered, or reflected [4]. Diffusive reflection light from the surface is usually recorded to estimate material optical properties. The most common method is that performing a diffusion approximation of the Boltzmann radiation transfer equation, which describes the relationship between the diffusive light intensity and desired optical parameters [5]. There are several challenges in it, including the selection of initial values, long computation time, and poor convergence. Many researchers have tried to resolve these issues.

Farrell *et al* first reported the use of artificial neural networks (ANN) to estimate  $\mu'_t = \mu_a + \mu'_s$  and  $\mu_{eff} = (3\mu_a\mu'_t)^{1/2}$  from reflective data obtained from a diffusive transportation model [6]. Chen *et al* used measurement data of spatial diffusive reflection to train an ANN to estimate  $\mu_a$  and  $\mu'_s$  [7]. Similarly, Warncke *et al* and Chen *et al* estimated  $\mu_a$  and  $\mu'_s$  values with ANNs [8, 9]. There is a lack of research on estimating the



**Figure 1.** Illustration of the fate of photons and diffusive reflection intensity profiles at different distances from the material surface.

four optical properties ( $\mu_a$ ,  $\mu_s$ ,  $g$ , and  $n$ ) simultaneously. It is known that the performance of estimation algorithms may drop quickly when the number of estimated parameters increases. The application of ANN has helped resolve the issue of computation speed, but few attempts have been made to enhance data richness to make estimation performance more robust. Thus, there is a need to enhance data richness when estimating multiple optical properties.

Optical properties affect the exit angles of diffusive reflection photons emitted from the surface [10]. In conventional measurements, this angle information is omitted when the diffusive reflection light intensity is only recorded at one distance from the surface (usually right at the surface). When it is applied to the estimation of optical parameters, the data richness would be enhanced because photon emission angles affect the light intensity distribution, which may make the diffusive light intensities at different distances from the material surface linearly independent. In this work, we proposed a back propagation (BP) neural network method [11–13] to determine material optical properties from diffusive reflection light intensity profiles obtained at multiple distances.

## 2. Method development

To enhance optical property estimation, the developed BP neural network based method includes the steps as described below.

Step 1: Obtain diffusive light intensities at multiple distances

When photons are incident in a medium, it will be scattered, reflected, or absorbed as shown in figure 1. In existing research, spatially-resolved diffusive reflection is measured at or near the surface. The photon exit angle is thus inconsequential and the information is not taken advantage of. In order to enhance data richness, we propose to capture diffusive light intensity profiles at multiple distances from the surface as illustrated in figure 1.  $\Delta h$  in figure 1 denotes the distance between two neighboring positions.

Monte Carlo (MC) simulations have been proven to be an effective method to simulate light propagation in medium [14, 15]. To demonstrate the method developed in this work, diffusive reflection intensity profiles at different distances from the material surface for various combinations of  $\mu_a$ ,  $\mu_s$ ,  $g$ , and  $n$  were simulated by MC simulation. To make the simulations more realistic, a Gaussian noise with different signal-to-noise ratios (SNR) was added to study the robustness of the method. In this work, flat surface was used to demonstrate the proposed concept, which was realized by a neural network in the following steps 3 and 4. BP neural networks are not limited by the shape of surfaces. The neural network can be trained with the data from any surfaces with any shape and roughness. If data were too uncertain because of too complex shapes or roughness, other methods will also have problems to estimate parameters. In reality, flat surfaces themselves have wide applications for material properties measurement, for example, milk quality, oil quality, blood, and many others.

Step 2: Features extraction

Direct use of reflection intensity profiles is computationally inefficient. Hence, effective data reduction is needed [16–18]. In this work, the following features were extracted: (1) Correlation, (2) Contrast, (3) Energy, (4) Homogeneity, and (5) Second moment. These features were selected experimentally based on their usefulness in predicting the optical properties.

### Step 3: Neural network training and testing

A BP neural network was used to estimate  $\mu_a$ ,  $\mu_s$ ,  $g$ , and  $n$  from the intensity profile features. The MC simulation in *Step 1* provided the training and test data sets. The trained BP neural network consisted of four layers: an input layer, two hidden layers, and an output layer. The input to the BP neural network included the five feature vectors extracted from the reflection intensity profiles at multiple distances and the outputs are the four optical parameters.

By experimenting different network structures, the number of nodes in the first and second hidden layers was set at 9 and 14, respectively. The log-sigmoid activation function was selected for all the neurons. Several initialization methods for weights and thresholds were tested and results showed that the Gaussian random initialization method [19, 20] performed the best. The Levenberg-Marquardt training method [21, 22] was used in adjusting the weights and offsets in the backpropagation training process.

### Step 4: Application of the trained BP neural network.

After a BP neural network is trained and tested, it can serve as an optical property estimator. To use the estimator, the multiple diffusive reflection intensity profiles at multiple distances as illustrated in figure 1 are needed, and the intensity profile features as input vectors to the neural network are extracted.

## 3. Results and discussion

### 3.1. Generation of diffusive reflection intensity profiles at different distances from the material surface

The model for MC simulation in Wang *et al* [23] was adopted and used to generate reflection intensity profiles. The ranges of optical property values were found in [24]. In the simulations,  $\mu_a$  was assigned as a random number between  $0.1 \text{ cm}^{-1}$  and  $100 \text{ cm}^{-1}$ .  $\mu_s$  was assigned as a random number between  $200 \text{ cm}^{-1}$  and  $1800 \text{ cm}^{-1}$ . For the isotropy factor  $g$ , total forward scattering means  $g = 1$  and isotropic scattering means  $g = 0$ . For most biological materials in the visible and near-infrared regions, the values of  $g$  range from 0.69 to 0.99. In this work, it was assigned as a random number between 0.65 and 1. The refractive index  $n$  was assigned as a random number between 1 and 4. After the four random optical parameters are generated, they will be provided to the Monte Carlo algorithm to drive the simulation. Different levels of noise were added to these reflection intensity profiles.

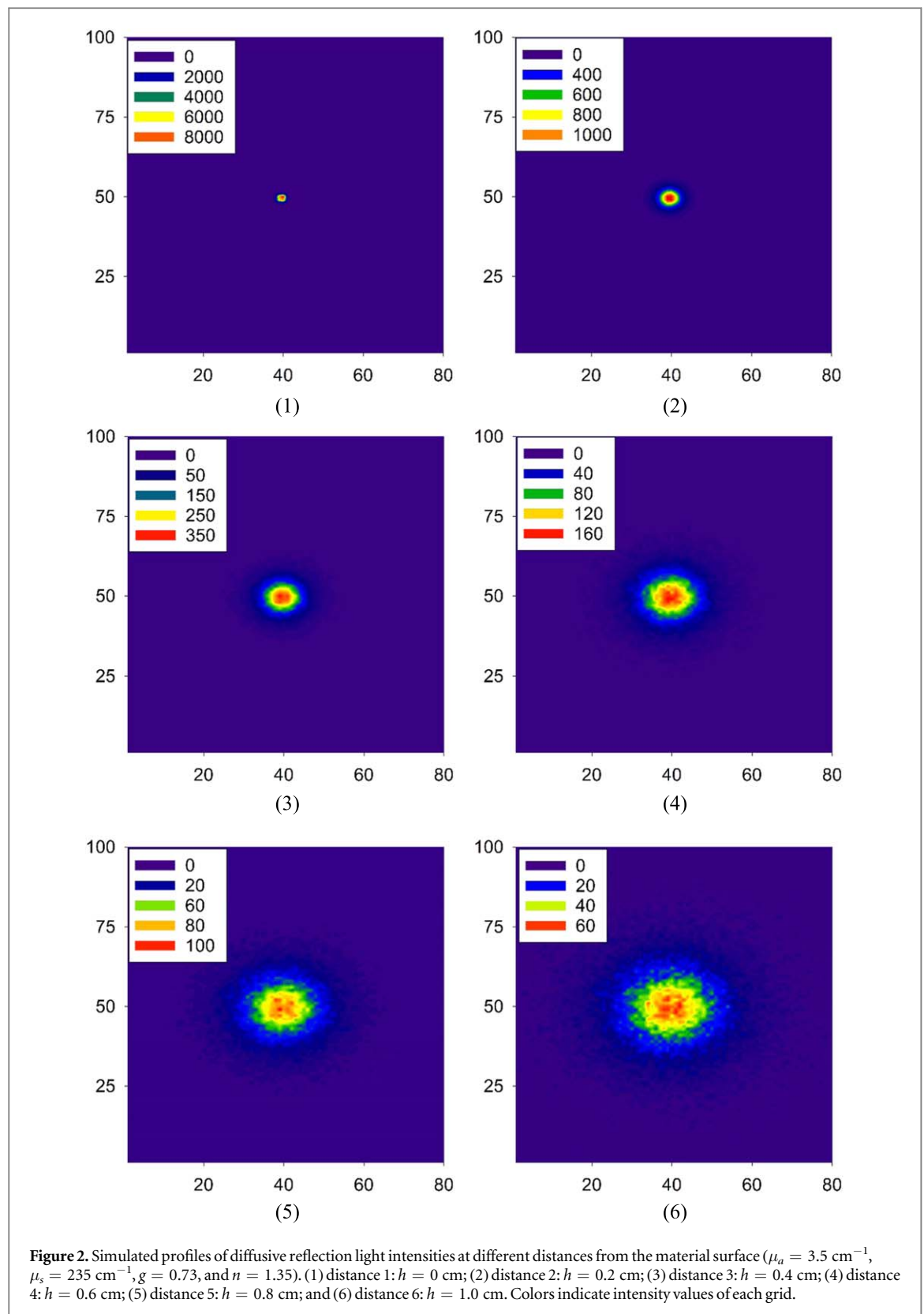
The photons were incident orthogonally on the material at a point. The position of photon was specified by the Cartesian coordinates  $(x, y, z)$ . The photon direction was specified by unit vector,  $\mathbf{r}$ , which can be equivalently described by the directional cosines  $(\mu_x, \mu_y, \mu_z)$ :  $\mu_x = \mathbf{r} \cdot \mathbf{x}$ ,  $\mu_y = \mathbf{r} \cdot \mathbf{y}$ , and  $\mu_z = \mathbf{r} \cdot \mathbf{z}$ , where  $\mathbf{x}$ ,  $\mathbf{y}$ , and  $\mathbf{z}$  are unit vectors along each axis. The photon position was initialized as  $(0, 0, 0)$  and the directional cosines were initialized as  $(0, 0, 1)$ . The photon location and direction were continuously updated according to the propagation rules. When a photon leaves the surface resulting from back diffusive reflection, its position  $(x_0, y_0, 0)$ , direction  $(\mu_x, \mu_y, \mu_z)$ , and weight were recorded. For an intersecting surface at distance  $h$  from  $z = 0$  (i.e. material surface), a photon emitted from  $z = 0$  would hit the surface  $z = h$  at  $(x_h, y_h, h)$ , where  $x_h = x_0 + \mu_x h / \mu_z$  and  $y_h = y_0 + \mu_y h / \mu_z$ . In this work, layers at equal increment  $\Delta h$  (0.2 cm) were used, so  $h = i \Delta h$  ( $i$  is a positive integer). For the  $\Delta h$  selection, it is not necessarily 0.2 cm, which is only used as an example to demonstrate the proposed method in this work. The neural network can be trained with data from any distances as long as the distance is not so far that the signal is too weak.

Figure 2 shows the profiles of diffusive reflection light intensities at different distances from the material surface for  $\mu_a = 3.5 \text{ cm}^{-1}$ ,  $\mu_s = 235 \text{ cm}^{-1}$ ,  $g = 0.73$ , and  $n = 1.35$ . There are  $80 \times 100$  grids ( $0.05 \text{ cm} \times 0.05 \text{ cm}$ ) for each intensity profile. The reflectance intensity (number of photons) is recorded for each grid. It shows that the photons gradually spread with increasing distance from the surface.

### 3.2. Intensity profile independence

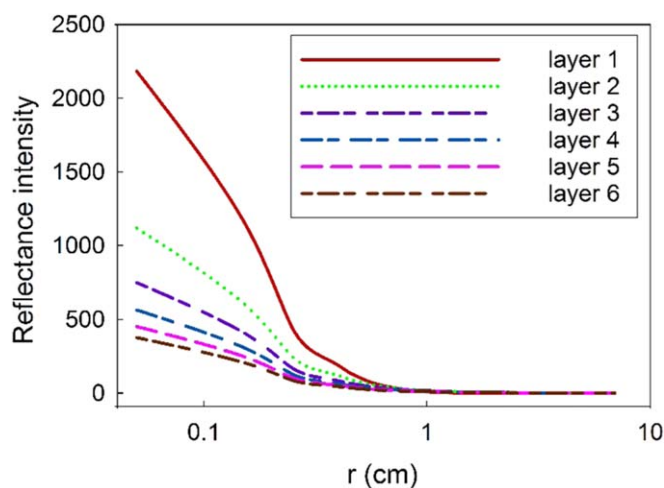
The six intensity profiles at different distance are independent to each other. To test the independence among the six intensity profiles, reflectance intensity was plotted as a function of radius  $r$  from the incident light location. Figure 3 shows the diffusive reflection intensity corresponding to the six intensity profiles in figure 2. It is obvious that the curves are not parallel. When the reflectance intensity vectors are put into a matrix  $A$ , the rank of  $A$  is 6, which means that these curves and the intensity profiles in figure 2 are independent. Since these vectors are not orthogonal to each other, the correlation between them will not be 0. They are independent. Each of them cannot be linearly represented by others, so they provide complementary information for determining optical properties.

The influence of Gaussian noise at different SNRs on the original intensity profile was tested. A Gaussian noise at SNR from 10 dB to 80 dB was added to the intensity profiles before further analysis, including intensity profile feature extraction, neural network training and testing.

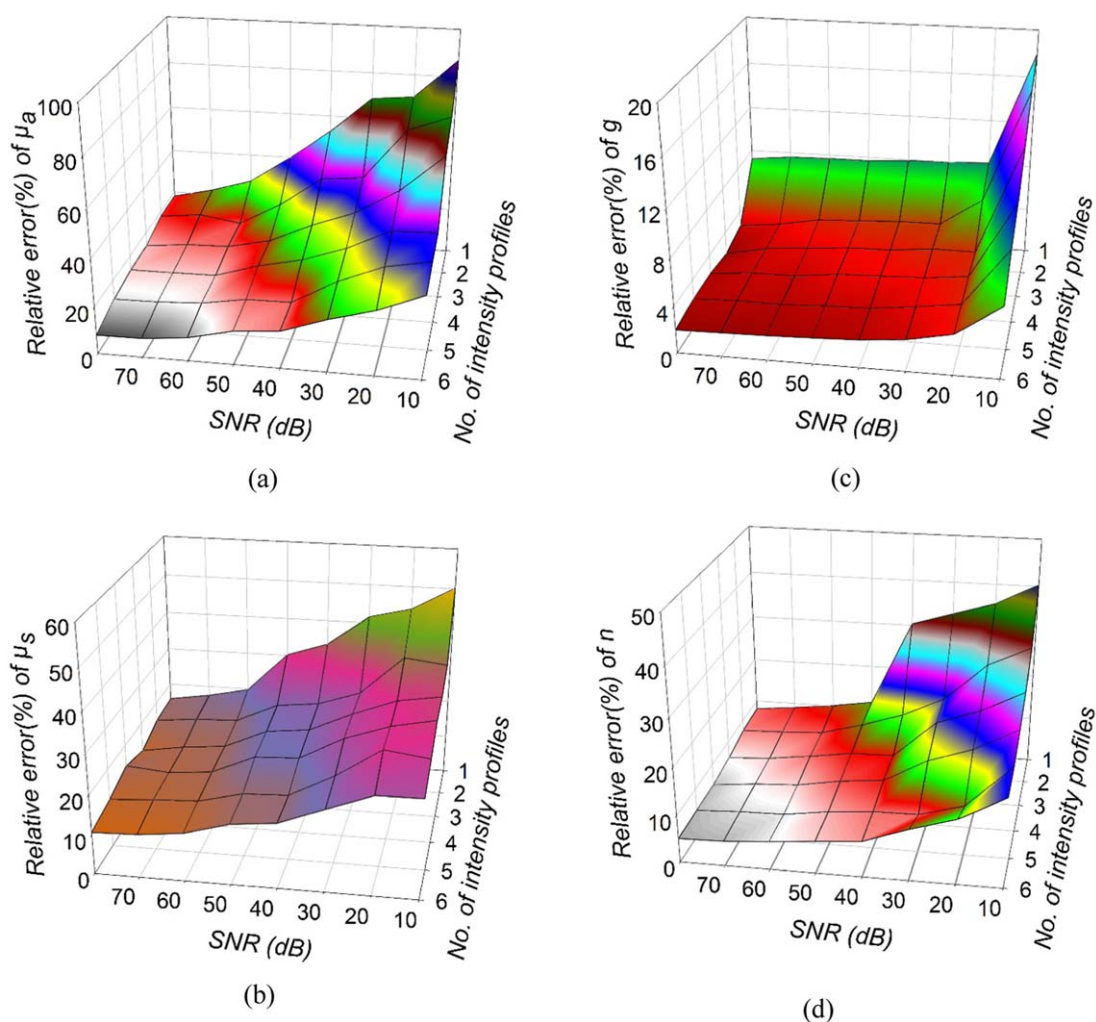


### 3.3. Optical property estimation

For each level of noise, there were totally 3,000 sets of intensity profile feature vectors (18,000 intensity profiles in total), of which 2,700 sets were used as training data and 300 sets were used as test data. Figures 4(a)–(d) show the average relative errors of the four estimated optical parameters changing with SNR and the number ( $m$ ) of intensity profiles taken at different distances from the surface of the material for the test dataset. Figure 4 clearly shows that the optical parameters estimated from a greater number ( $m$ ) of intensity profiles are more accurate and robust against noise. For example, when SNR is 40 dB, the mean relative errors (MRE) in  $\mu_a$ ,  $\mu_s$ ,  $g$ , and  $n$  for



**Figure 3.** Diffusive reflection light intensities of each grid as a function of radius  $r$  from the incident light at different distances from the material surface.



**Figure 4.** The mean relative errors of estimated optical properties as a function of SNR and the number of intensity profiles used as input: (a) absorption coefficient  $\mu_a$ , (b) scattering coefficient  $\mu_s$ , (c) anisotropy coefficient  $g$ , and (d) refractive index  $n$ .

the test data set were 8.5%, 10.1%, 2.3%, and 5.7%, respectively, if intensity profiles at six distances were used; while the MREs became 39.5%, 32.6%, 13.8%, and 6.8%, respectively if intensity profile at only one distance was used. This clearly demonstrates that measurements at more distances contribute to parameter estimation. More



independent data provide extra constraints for model parameter estimation and make model parameter more robust. This is a universal mathematical solution. The proposed BP neural network may be retrained to take care of other noises in future research.

The traditional least squares method for estimating the optical properties was tested for comparison. The method uses the Boltzmann transfer equation to fit the spatial diffusive reflection curve to derive  $\mu_a$  and  $\mu'_s$ . The estimation may fail to converge although only two optical properties were estimated. For example, the theoretical diffusive light intensity was generated through MC simulation for  $\mu_a = 3.5 \text{ cm}^{-1}$ ,  $\mu_s = 235 \text{ cm}^{-1}$ ,  $g = 0.73$ , and  $n = 1.35$ . The true  $\mu'_s$  was  $63.45 \text{ cm}^{-1}$ . In one least squares fitting, the algorithm converged to  $\mu_a = 3.1 \text{ cm}^{-1}$  and  $\mu'_s = 56.64 \text{ cm}^{-1}$ ; in another least squares fitting, the algorithm converged to  $\mu_a = 20.46 \text{ cm}^{-1}$  and  $\mu'_s = 0.016 \text{ cm}^{-1}$ . For the two fittings, no noise was added to the simulated theoretical diffusive reflection light intensity. This clearly shows that although the fittings are good, the parameters obtained can be totally wrong.

Different from the method proposed in this work, the prediction of optical properties by the traditional nonlinear least squares inverse algorithm was affected significantly by the initial values. The diffusive light intensity at the material surface follows a simple decay with distance from the incident light point, which does not provide rich dynamic information. In the traditional least squares algorithms, initial values should be provided, which highly affect the performance of the algorithms. If we do not know the range of the values, it would be very difficult to provide suitable initial values. An inappropriate initial value may lead big error in parameter estimation. Without experience about the optical property of materials, it is difficult to judge whether an estimated optical parameter from the traditional least square algorithms is valid.

## 4. Conclusions

To improve optical property estimation from diffusive reflection measurement, a method was developed in this work which uses diffusive light intensity profiles obtained at different distances from the material surfaces to enhance data richness. The backpropagation neural network algorithm was used to estimate the  $\mu_a$ ,  $\mu_s$ ,  $g$ , and  $n$  at the same time without needing close initial values as the traditional least squares algorithms usually require. The proposed method is robust against noise and the relative errors for  $\mu_a$ ,  $\mu_s$ ,  $g$ , and  $n$  were less than 10% respectively when the noise level was at 40 dB.

## Acknowledgments

This project is partially supported by National Natural Science Foundation of China (No: 31771680, No: 51961125102, No: 21706096), Fundamental Research Funds for the Central Universities of China (No: JUSRP51730A), the Natural Science Foundation of Jiangsu Province (No: BK20160162), the Modern Agriculture Funds of Jiangsu Province (No: BE2018334), the 111 Project (B12018), and the Research Funds for New Faculty of Jiangnan University.

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