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A two-step parameter optimization algorithm for improving estimation of optical properties using spatial frequency domain imaging

Dong Hu[a,c], Renfu Lu[b,*], Yibin Ying[a,d,*]

[a] College of Biosystems Engineering and Food Science, Zhejiang University, 866 Yuhangtang Road, Hangzhou 310058, China
[b] USDA Agricultural Research Service, 524 S. Shaw Lane, East Lansing, MI 48824, USA
[c] Department of Biosystems and Agricultural Engineering, Michigan State University, 524 S. Shaw Lane, East Lansing, MI 48824, USA
[d] Zhejiang A&F University, Hangzhou, Zhejiang 311300, China

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ABSTRACT

This research was aimed at optimizing the inverse algorithm for estimating the optical absorption (μ_a) and reduced scattering (μ_s') coefficients from spatial frequency domain diffuse reflectance. Studies were first conducted to determine the optimal frequency resolution and start and end frequencies in terms of the reciprocal of mean free path ($1/mfp'$). The results showed that the optimal frequency resolution increased with μ_s' and remained stable when μ_s' was larger than 2 mm^{-1}. The optimal end frequency decreased from $0.3/mfp'$ to $0.16/mfp'$ with μ_s' ranging from 0.4 mm^{-1} to 3 mm^{-1}, while the optimal start frequency remained at 0 mm^{-1}. A two-step parameter estimation method was proposed based on the optimized frequency parameters, which improved estimation accuracies by 37.5% and 9.8% for μ_a and μ_s', respectively, compared with the conventional one-step method. Experimental validations with seven liquid optical phantoms showed that the optimized algorithm resulted in the mean absolute errors of 15.4%, 7.6%, 5.0% for μ_a and 16.4%, 18.0%, 18.3% for μ_s' at the wavelengths of 675 nm, 700 nm, and 715 nm, respectively. Hence, implementation of the optimized parameter estimation method should be considered in order to improve the measurement of optical properties of biological materials when using spatial frequency domain imaging technique.

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1. Introduction

Light absorption and scattering are two basic phenomena during the interaction of light with biological tissues, which are characterized by the absorption coefficient (μ_a) and reduced scattering coefficient (μ_s'). Measurement of the optical properties has been an important subject of research, because they are related to the chemical and structural properties of biological tissues [1–3]. Moreover, quantification of the tissue optical properties can help us in understanding light propagation in biological tissues, better interpreting the measured optical data, optimizing optical devices, and improving food quality and safety assessment.

During the past decades, different optical techniques, including spatially-resolved (SR), time-resolved, frequency domain, and spatial frequency domain imaging (SFDI), have been developed to measure the optical properties of biological materials by using inverse algorithms for the diffusion approximation equation (DAE) [4]. As a relatively new optical technique, SFDI has advantages over other optical methods because it can provide quantitative two or three-dimensional mapping of the optical absorption and reduced scattering coefficients for biological materials. With this method, diffusely back-scattered images are captured from a turbid sample subjected to the illumination of sinusoidal pattern with different spatial frequencies (f_x). The tissue optical properties are then determined by fitting the demodulated reflectance on a pixel-by-pixel basis using an analytical solution of the diffusion model derived by Cuccia et al. [5]. The analytical solution is derived based on two important assumptions that scattering is dominant in the tissues (i.e., $\mu_s' >> \mu_a$), and the spatial frequency of sinusoidal pattern is much smaller than the transport coefficient ($\mu_{tr} = \mu_a + \mu_s'$). While SFDI technique is promising for optical characterization of biological materials over a large area, there still exist considerable difficulties in accurate estimation of the optical properties due to errors associated with signal acquisitions in real applications and the complex inverse parameter estimation algorithm. Efforts have thus been made to investigate the relationship between the

* Corresponding authors.
E-mail addresses: hudong@msu.edu (D. Hu), renfu.lu@ars.usda.gov (R. Lu), yingyb@zju.edu.cn (Y. Ying).

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spatial frequency and optical properties in order to improve the estimation accuracy [5,6]. Hu et al. [7] modeled light propagation in turbid media under the normal incidence of sinusoidal illumination using finite element method. They recommended that the values of μ_s'/μ_a and μ_{tr}/f_x should be larger than 10 and 3 respectively, so that the contributions of sub-diffuse reflectance to the diffuse reflectance at the surface of the sample become negligible, which would, in turn, result in more accurate prediction of diffuse reflectance. In a conventional approach, μ_a and μ_s' for a sample are estimated simultaneously from the diffuse reflectance profiles, using an inverse nonlinear least squares algorithm with the same frequency resolution and same start and end frequencies for all samples. Hereinafter we refer to this estimation method as 'conventional one-step method', compared to the 'two-step method' proposed in this paper. However, the optical properties estimated by the conventional one-step method with the fixed frequency range (including frequency resolution and start and end frequencies) are often less accurate because no a priori knowledge is available about the sample, and it is thus difficult to select optimal spatial frequencies with respect to μ_{tr}. Studies have been reported of using the SFDI technique with different spatial frequency regions. Anderson et al. [8] used nine equally-spaced spatial frequencies from 0.0149 mm^{-1} to 0.1344 mm^{-1} for estimating the optical properties of normal and bruised apple tissues, while Mazhar et al. [9] only utilized five spatial frequencies from 0 to 0.2 mm^{-1} for the measurement of thermal burns in a porcine model. To measure the μ_a and μ_s' of liquid optical phantoms, Cuccia et al. [5] used 30 spatial frequencies between 0 and 0.13 mm^{-1}. The spatial frequency regions used in these reported studies were fixed, largely based on their own preliminary studies. Furthermore, the optical properties of biological materials vary from sample to sample, which would cause more difficulties for selection of spatial frequencies. Although SFDI has been used for determination of optical properties of food and biological materials, such as apple, mouse, porcine and human ovarian [9–12], no study has been reported on optimizing the spatial frequency resolution and start and end frequencies for better estimation of optical properties.

Therefore, the overall objective of this research was to optimize the inverse parameter estimation algorithm, so that more accurate and reliable optical property estimations of biological materials can be made by using the SFDI technique. The specific objectives were to:

- Optimize the spatial frequency resolution and start and end frequencies for the inverse nonlinear parameter estimation algorithm;
- Propose a new two-step method for estimation of the absorption and scattering properties; and
- Validate the optimized inverse parameter estimation algorithm using liquid optical phantoms of known optical properties.

2. Materials and methods

2.1. Diffusion model for spatial frequency domain imaging technique

The light transfer in a turbid medium is governed by the radiative transfer equation (RTE), which is based on the principle of conservation of energy [13]. For most biological materials, light scattering is dominant over absorption (i.e., $\mu_s' >> \mu_a$); hence, the DAE, which is a simplified form to the RTE, is adequate to model light propagation in tissues. Consider a homogeneous, linear scattering medium of semi-infinite geometry normally incident at its surface by a steady-state illumination of one-dimensional planar, sinusoidal pattern, the DAE can be expressed as

$$\nabla^2\varphi(x,z) - \mu_{eff}'^2\varphi(x,z) = -3\mu_{tr}S. \quad (1)$$

where $\varphi(x, z)$ is the fluence rate, in which x represents the horizontal axis, along which the illumination pattern changes sinusoidally and z represents the depth from the surface of the semi-infinite medium, $\mu_{eff}' = (3\mu_a\mu_{tr} + (2\pi f_x)^2)^{1/2}$ is the scalar attenuation coefficient, $\mu_{tr} = \mu_a + \mu_s'$ is the transport coefficient, f_x is the spatial frequency, and S is the planar illumination. By modeling the illumination in Eq. (1) as an extended source term that decays exponentially with the depth [14], and applying the partial current boundary condition along the physical boundaries [15], the diffuse reflectance $R(f_x)$ at the surface can be expressed as follows [5]:

$$R(f_x) = \frac{3Aa'}{\left(\mu_{eff}'/\mu_{tr} + 1\right)\left(\mu_{eff}'/\mu_{tr} + 3A\right)}. \quad (2)$$

where $A = \frac{1-R_{eff}}{2(1+R_{eff})}$ is the proportionality constant, $R_{eff} \approx 0.0636n + 0.668 + 0.71/n - 1.44/n^2$ is the effective reflection coefficient, n is the refractive index of the medium, and $a' = \mu_s'/\mu_{tr}$ is the reduced albedo. In this study, Eq. (2) was used for inversely estimating μ_a and μ_s' via a nonlinear curve-fitting algorithm from diffuse reflectance profiles, which were either generated by Monte Carlo simulation or demodulated through experimental data.

2.2. Monte Carlo simulation

Monte Carlo (MC) simulation, as a category of stochastic numerical methods, has been widely used for modeling light propagation in tissues [16,17]. Because of its high accuracy, the method is often viewed as a gold standard, and the forward prediction of diffuse reflectance are frequently used as the reference to verify the effectiveness of other methods. However, since the MC method is time-consuming and cannot separate μ_a and μ_s' perfectly [18,19], it is not suitable to solve inverse problems for fast determination of optical properties.

In this study, a publicly available MC program developed by Wang et al. [20] was used for generating diffuse reflectance profiles of 40 samples with different combinations of μ_a and μ_s', as shown in Table 1. The optical property values for these samples were chosen based on previous studies, covering a large range of biological materials with 0.004 $mm^{-1} \le \mu_a \le 0.3$ mm^{-1}, 0.4 $mm^{-1} \le \mu_s' \le 3$ mm^{-1} and $10 \le \mu_s'/\mu_a \le 100$ [21–23]. It should be mentioned that $1/mfp'$ was treated as the reference unit for optimization of the spatial frequency. In the MC simulation, a package of 5×10^6 photons were tracked. The maximum radial distance of the medium was set to 50 mm, which is large enough to be treated as semi-infinite. The spatial resolution for both radial distance and depth was set to 0.1 mm. The refractive index of the medium was chosen to be 1.35, which is typical for many biological materials [24,25]. To simulate the diffuse reflectance under the illumination of sinusoidal pattern, the steady-state SR diffuse reflectance profiles along the radial distance under the normal incidence of an infinite small light source were first generated for every sample. The diffuse reflectance under the sinusoidal pattern of illumination for different spatial frequencies was then obtained by using the one-dimensional Hankel transform of order zero, as shown in Eq. (3):

$$R(f_x) = \sum_{i=1}^{n} r_i J_0(f_x r_i) R(r_i) \Delta r_i. \quad (3)$$

where r is the radial distance in the SR method, and $J_0(f_x r_i)$ is the zeroth-order Bessel function of the first kind. The approach has been proven effective and accurate in previous studies [5,26] and our preliminary MC simulation study. The reflectance profiles generated using Eq. (3) were then used for optical property estimation and inverse algorithm optimization.