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Optical properties reconstruction using the adjoint method based on the radiative transfer equation

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ABSTRACT

An efficient algorithm is proposed to reconstruct the spatial distribution of optical properties in heterogeneous media like biological tissues. The light transport through such media is accurately described by the radiative transfer equation in the frequency-domain. The adjoint method is used to efficiently compute the objective function gradient with respect to optical parameters. Numerical tests show that the algorithm is accurate and robust to retrieve simultaneously the absorption μ_a and scattering μ_s coefficients for lowly and highly absorbing medium. Moreover, the simultaneous reconstruction of μ_s and the anisotropy factor g of the Henyey–Greenstein phase function is achieved with a reasonable accuracy. The main novelty in this work is the reconstruction of g which might open the possibility to image this parameter in tissues as an additional contrast agent in optical tomography.

1. Introduction

Diffuse Optical Tomography (DOT) is a non-invasive imaging modality which employs a visible or Near infrared (NIR) Laser source for probing biological tissues and measures light intensities at the boundary surface. In recent years, potential applications of DOT have been developed such as breast cancer detection [1] and brain functional imaging [2]. This technique seeks to recover the spatial distributions of optical properties inside the medium through an image reconstruction algorithm. Optical properties are different between healthy and cancerous tissues [3,4] due to physiological or pathological changes [5]. In spite of all the success of DOT in cancer diagnosis applications, to date, only absorption (μ_a) and reduced scattering (μ_s') coefficients reconstruction can be found in the literature. However, the anisotropy factor g of the Henyey–Greenstein (H-G) phase function has an important effect on light propagation [6] and can reveal rich informations on the anisotropic scattering behavior of the tissue: [7] showed that the g value of porcine brain tissue increases from 0.561 to 0.834 after thermal coagulation, [8] demonstrated that the anisotropy factor g of rat liver decreases from 0.952 to 0.946 in a tumor at 633 nm, [9] proved experimentally that g was different for normal human liver tissue and liver metastases at three different wavelengths. That means that g can also be modified when tissue is affected by an eventual tumor besides μ_a and μ_s. Therefore, this factor can provide a potential contrast agent for optical medical diagnosis between healthy and tumoral tissues. To our best knowledge, up to now, no works have been done to investigate the reconstruction of the spatial distribution of g [10]. On the other hand, an efficient forward model to predict light transport in the biological tissue is required in order to estimate optical parameters. Many research groups have adopted the diffusion equation (DE) as a forward model [11–13]. However, the DE model fails to accurately predict light propagation close to sources and boundaries, and also in highly absorbing mediums [14]. An additional drawback of the DE is that the estimation of g is not possible (g is assumed to be constant and known), due to the introduction of the reduced scattering coefficient and then the loss of information about the scattering phase function [6]. To overcome these limitations, more and more interest is turned towards a forward model based on the radiative transfer equation (RTE). The RTE rigorously describes the light propagation in biological tissues. The anisotropy factor g is an independant parameter in the RTE via the H-G phase function. Different forms of the RTE have been used in DOT. The frequency-domain (FD) approach [15–21] is the most widely employed, since it is a good trade-off between time-domain [22–24] and steady-state domain [25]. Moreover, the FD approach provides additional information (phase shift) compared to the steady-state modality and avoids the technical limitations of the experimental setup for time-domain often expensive. In addition, the use of FD data al-

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lows to better separate the optical properties than the steady-state data by reducing the crosstalk issue when simultaneous estimation is applied [16]. Another challenging task still remains in DOT: the inverse problem. The inversion algorithm can be considered as a large-scale optimization problem, since the optical properties vary spatially inside the medium. In principle, the simultaneous estimation of the three optical properties (μ_a, μ_s and g) is not possible, due to the non-uniqueness of the ill-posed problem when several optical properties distributions lead to an identical set of boundary data [6]. Additionally, these three parameters differ in nature, units, order of magnitude and sensitivities on the emerging intensity of the forward model which makes the estimation inextricable. That's why, in this work, we reconstructed only two parameters either (μ_a and μ_s) or (μ_s and g) simultaneously in order to reduce the ill-posed nature of the problem. This inversion aims at recovering the optical properties of tissue through the minimization of an appropriate objective function (OF). Most of the time, the OF is the least-square error norm between the measured and the predicted data calculated by the forward model. Gradient-based algorithms are commonly used as optimization methods [13,16,26], which employ the gradient of the OF with respect to the optical parameters to find the minimum. These methods proved to be efficient and robust in DOT [24]. On the other side, the core problem and difficulty in the inversion procedure is to accurately compute the gradient of the OF. This process can be computational-intensive due to the number of parameters to retrieve which are space dependent. Generally, the adjoint differentiation (AD) is the most commonly used method for calculating the gradient because it uses only elementary results at each iteration step of the forward model [27,28]. However, when the dimension of the problem is high (larger than 1000 for example), the use of the AD becomes cumbersome and computationaly expensive. More recently, [29] employed the adjoint method which gives an efficient and fast way to compute the OF gradient regardless of the number of unknowns. This is done by solving an additional (adjoint) equation for the adjoint variable whose computational cost is equivalent to that of the forward calculation.

In this work, a gradient-based algorithm using the RTE as forward model is employed to reconstruct the optical properties (μ_a, μ_s and g) of a heterogeneous medium. The gradient of the OF is obtained accurately by means of the adjoint method in the FD. The objective of this study is to test the efficiency and the robustness of the proposed algorithm in presence of some issues encountered in the DOT. These issues such as the collimated source number, the crosstalk between two optical parameters, the inclusion contrast level, the highly absorbing medium, the measurements noise level and the inclusion location effects are examined through several test cases. Furthermore, for author's best knowledge, the estimation of g and the simultaneous reconstruction of μ_s and g have not been reported yet in the previous works. This explains our motivation to test in particular the feasibility of the present method to reconstruct simultaneously μ_s and g with and without crosstalk. First, the RTE equations are described and the detector predictions on the boundary are given. Second, the adjoint method is presented through a lagrangian formalism for the computation of the OF gradient at multiple modulation frequencies. Finally, to illustrate the performance of the algorithm, single and simultaneous reconstructions of optical properties based on numerical test phantoms are presented in presence of certain issues mentioned above.

2. Forward model

In DOT, the light transport in the biological tissues is a forward model which aims at computing the prediction of the detectors reading once the source and the optical properties of the medium are known. The biological tissue is illuminated by an external collimated Laser beam $\Upsilon(\boldsymbol{r_s}, \omega_k)$ at the source position $\boldsymbol{r_s}$ on the surface. ω_k is the modulation frequency of the intensity-modulated Laser source. In order to take into account this collimated light, the energy arriving in the medium is separated into two components $\psi = \psi_c + \psi_s$, respectively the collimated ψ_c and scattered radiance ψ_s. The ψ_c radiance is governed by the RTE state equation $\mathcal{R}_c$ in the collimated direction $\boldsymbol{\Omega_c}$ and is solved analytically.

$$\mathcal{R}_c = \left[\boldsymbol{\Omega_c} \cdot \nabla + \left(\frac{i\,\omega_k}{v} + \mu_t(\boldsymbol{r}) \right) \right] \psi_c(\boldsymbol{r}, \omega_k) = 0. \tag{1}$$

The velocity of light, v, in tissue is the ratio $v = c/n$ of the velocity of light in vacuum and the refractive index of tissue. The total extinction coefficient $\mu_t(\boldsymbol{r})$, at position $\boldsymbol{r}$, is the sum of the absorption $\mu_a(\boldsymbol{r})$ and the scattering $\mu_s(\boldsymbol{r})$ coefficients. The boundary condition for the collimated component $\psi_c(\boldsymbol{r}, \omega_k)$ is given by:

$$\psi_c(\boldsymbol{r}, \omega_k) = \Upsilon(\boldsymbol{r_s}, \omega_k) \quad \text{for} \quad \boldsymbol{\Omega_c} \cdot \boldsymbol{n} < 0, \tag{2}$$

where $\boldsymbol{n}$ is the outward normal unit vector of the boundary. It should be noted that the component Y, in Eq. 2, represents only the transmitted part (no reflexion) of the collimated Laser beam into the medium. The scattered radiance $\psi_s(\boldsymbol{r}, \boldsymbol{\Omega}, \omega_k)$ is obtained by solving the RTE state equation $\mathcal{R}_s$ in the direction $\boldsymbol{\Omega}$ of the light propagation such as:

$$\mathcal{R}_s = \left[\boldsymbol{\Omega} \cdot \nabla + \left(\frac{i\,\omega_k}{v} + \mu_t(\boldsymbol{r}) \right) \right] \psi_s(\boldsymbol{r}, \boldsymbol{\Omega}, \omega_k) - \mu_s(\boldsymbol{r}) \times \int_{\Omega'=2\pi} p(\boldsymbol{\Omega'}, \boldsymbol{\Omega})\ \psi_s(\boldsymbol{r}, \boldsymbol{\Omega'}, \omega_k)\ d\Omega' - S_c(\boldsymbol{r}, \boldsymbol{\Omega}, \omega_k) = 0. \tag{3}$$

The H-G phase function $p(\boldsymbol{\Omega'} \cdot \boldsymbol{\Omega})$ is the most widely adopted scattering phase function in biomedical optics and has been used here [23,30]. This function, is the probability that photons traveling in direction $\boldsymbol{\Omega'}$ scatter into direction $\boldsymbol{\Omega}$. The H–G phase function mathematical expression in 2D is given by:

$$p(\boldsymbol{\Omega'} \cdot \boldsymbol{\Omega}) = \frac{1}{2\pi} \frac{1 - g^2(\boldsymbol{r})}{\left(1 + g^2(\boldsymbol{r}) - 2\ g(\boldsymbol{r})\ \boldsymbol{\Omega'} \cdot \boldsymbol{\Omega}\right)}. \tag{4}$$

The anisotropy factor $g(\boldsymbol{r})$ represents the mean cosine of the angles of the scattered directions $\boldsymbol{\Omega}$ with respect to the incident ones $\boldsymbol{\Omega'}$. This factor is spatially dependent in our case for the heterogeneous medium. The source term $S_c(\boldsymbol{r}, \boldsymbol{\Omega}, \omega_k)$ in Eq. 3 induced by the scattering of the collimated radiance $\psi_c(\boldsymbol{r}, \omega_k)$ is given by:

$$S_c(\boldsymbol{r}, \boldsymbol{\Omega}, \omega_k) = \mu_s(\boldsymbol{r})\ p(\boldsymbol{\Omega_c}, \boldsymbol{\Omega})\ \psi_c(\boldsymbol{r}, \omega_k). \tag{5}$$

Eq. (3) is associated to a semi-transparent boundary condition [31] with Fresnel reflection at the interface (air / biological tissue) due to the refractive index mismatch. The detector prediction $P(\boldsymbol{r_d}, \omega_k)$ corresponding to the exitance at the detector position $\boldsymbol{r_d}$ on the illuminated surface is obtained by:

$$P(\boldsymbol{r_d}, \omega_k) = \int_{\boldsymbol{n} \cdot \boldsymbol{\Omega'} > 0} \left[1 - \rho(\Theta)\right]\ \psi_s(\boldsymbol{r}, \boldsymbol{\Omega'}, \omega_k)\ \left(\boldsymbol{\Omega'} \cdot \boldsymbol{n}\right)\ d\Omega', \tag{6}$$

where $\rho(\Theta)$ is the reflectivity of the surface $\partial\mathcal{D}$. The forward model has been solved accurately with a Modified Finite Volume Method (MFVM). The methodology of this method is not repeated here and we refer the reader to [32], for details. The stability and accuracy of the MFVM have been validated through comparisons with the Monte Carlo (MC) technique and analytical solution of RTE on available test cases. The MFVM, compared to other deterministic numerical solutions of the RTE (available in the literature) has the advantage to have a high precision with an error less than 1% with respect to MC simulations and RTE analytical solution. This is mainly due to the fact that the RTE is also solved inside each control volume through an exponential schema.