# Fast Monte Carlo inversion for extracting the optical properties of tubular tissues

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Reconstruction of absorption coefficient $\mu_a$ and scattering coefficient $\mu_s$ is very important for applications of diffuse optical tomography and near infrared spectroscopy. Aiming at the early cancer detection of cervix and stomach, we present a fast inverse Monte-Carlo scheme for extracting $\mu_a$ and $\mu_s$ of a tubular tissue from the measurement on frequency domain. Results show that the computation time for reconstructing one set of $\mu_a$ and $\mu_s$ is less than 1 min and the relative errors in reconstruction are less than $\pm 10\%$ for the optical properties of normal cervical tissue and precancerous lesions.

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Determination of tissue optical properties is a significant topic in tissue optics[1−3]. Measurement of absorption coefficient $\mu_a$ and scattering coefficient $\mu_s$ in near infrared (NIR) can be carried on frequency domain (FD) where the intensity of NIR light incident on a sample is modulated in radio frequency and the diffusely reflected or transmitted signal is measured with a phase-sensitive detection system. Sinusoidally intensity-modulated light propagates, through the turbid sample, forming photon density waves (PDWs). Wave dispersion is highly dependent on the optical properties of the sample. Thus, measurements of the amplitude attenuation and phase delay of PDW can be used to derive $\mu_a$ and $\mu_s$. Because of the nonlinear nature of the inverse problem for deriving $\mu_a$ and $\mu_s$, the reconstruction is commonly achieved in an optimization procedure, i.e., the output from the forward model is updated until the difference between the measurement and this output is acceptable. For cases of practical interest, e.g., the endoscopic imaging using NIR light, the photon migration cannot be adequately described by diffusion equation, and Monte Carlo (MC) simulation is the preferred model. However, the applicability of MC simulations is limited by the long computation time necessary to obtain statistically reliable results. In an update procedure, many separate and independent forward calculations have to be run, thus, the rapid forward MC calculation will be the key point for $\mu_a$ and $\mu_s$ reconstruction. For example, if separate MCs are adopted in the reconstruction and 10 iterations are needed to approach converge, the computation time will be more than 40 h for $10^7$ initial emitting photons. Until now, the developed speeding strategies of forward MC calculation include the perturbation MC[4], and the condensed MC[5], etc. However, the former is not only sensitive to the variation in scattering coefficient $\mu_s$ but also time consuming (about 30 min to complete the reconstruction), while the latter is only applicable to the semi-infinite medium or infinite slab.

This article aims at the development of the inverse MC for rapid extraction of $\mu_a$ and $\mu_s$ of tubular organ such as the cervix and the stomach with the FD measurement. The method is illustrated in Fig. 1, which includes strategies in both the construction of a FD MC database and the obtainment of FD information at any $\mu_a$ and $\mu_s$.

Considering the structure of a cervix, the tissue model adopted is a homogenous pipe with the inner hole and outer boundary in diameters of 2 and 4 cm, respectively[6]. The anisotropic parameter $g$ and the relative refractive index of the tissue are assumed to be 0.9 and 1.33, respectively. The separation between the source and detection location is 1.0 cm. The number of the initial emitting photons in MC is $10^7$. It has been reported that, for normal cervical tissue at 811-nm wavelength, $\mu_a$ is from 0.18 to 0.36 $cm^{-1}$ and $\mu_s$ is from 45 to 67 $cm^{-1}$, respectively. For precancerous lesions (CIN II), $\mu_a$ is in the range of 0.15 to 0.29 $cm^{-1}$ and $\mu_s$ is $41 - 57$ $cm^{-1}$. For carcinoma *in situ* (CIN III), although $\mu_a$ is in the same range to CIN II but $\mu_s$ decreases to $35 - 50$ $cm^{-1}$[7]. Concerning the reported optical properties of other biological tissues[8], the optical properties for constructing the MC database are selected as $\mu_a = 0.05 - 0.60$ $cm^{-1}$ and $\mu_s = 30 - 150$ $cm^{-1}$.

The construction of MC database follows three steps.

Step 1: For $\mu_a = 0$, independent time domain (TD) MC simulations are carried out while $\mu_s$ is in the above range and with a step of 10 $cm^{-1}$.

Step 2: Although Fourier transform (FT) method can be used to get the frequency information from temporal profiles possibly calculated from TD MC, it involves large numbers of floating point operations and its

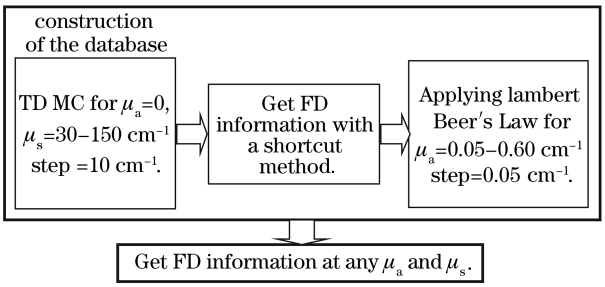


Fig. 1. Flowchart of the forward calculation.

 

accuracy depends on the selection of the time window. In this letter, a shortcut method is adopted which only needs the weight $W_k$ and the mean flight time $t_k$ of the $k$th photon package in TD MC. When only one modulation frequency $\omega_0$ is utilized in measurement, the FD information can be expressed as[6]

$$\tilde{u}_{\rm sc}(\omega_0) = \sum_k W_k \exp(i\omega_0 t_k). \quad (1)$$

The imaginary and real components of $\tilde{u}_{\rm sc}$ provide the amplitude $A$ and phase $\phi$ of PDW for the extraction of optical properties.

Step 3: To continue the database for $\mu_{\rm a} \neq 0$, Lambert Beer's Law is adopted[9]. If $l_k$ is the mean path length of a photon package which equals to the product of $t_k$ and the speed of light in tissue, then the new photon weight $w'_k$ can be obtained through multiplying the corresponding photon weight at $\mu_{\rm a} = 0$ by $\exp(\mu_{\rm a} l_k)$.

After the aforementioned procedure, a database of $A$ and $\phi$ is built while $\mu_{\rm a}$ is from 0.05 to 0.60 $\rm cm^{-1}$ with a step of 0.05 $\rm cm^{-1}$ and $\mu_{\rm s}$ is from 30 to 150 $\rm cm^{-1}$ with a step of 10 $\rm cm^{-1}$.

The reconstruction follows Levenberg-Marquardt (LM) optimization to minimize the difference between the real $y = \{A, \phi\}$ and $\hat{y} = \left\{\hat{A}, \hat{\phi}\right\}$ calculated with MC. The iteration step is given by[10]

$$p_{n+1} = p_n + [J^{\rm T} J + \lambda I]^{-1} J^{\rm T} \Delta y, \quad (2)$$

where $p = \{\mu_{\rm a}, \mu_{\rm s}\}$, $J$ is the Jacobian matrix of the forward calculation, $\lambda$ is a regularization parameter, and $\Delta y = y - \hat{y}$.

Since MC simulations under any $\mu_{\rm a}$ and $\mu_{\rm s}$ are needed in the optimization procedure, the database constructed above has to be extended dynamically during the reconstruction. As can be seen from Fig. 2, $A$ and $\phi$ change smoothly with $\mu_{\rm a}$ and $\mu_{\rm s}$, which means that it is possible to use polynomial fitting and interpolation to obtain the desired $A$ and $\phi$ at any $\mu_{\rm a}$ and $\mu_{\rm s}$ in this range. For two-element polynomial interpolation, the polynomial fitting is expressed as

$$\begin{aligned} A(\mu_{\rm a}, \mu_{\rm s}, n) &= \left(a_0 + a_1 \mu_{\rm a}^1 + \cdots + a_n \mu_{\rm a}^n\right) \\ &\quad \times \left(b_0 + b_1 \mu_{\rm s}^1 + \cdots + b_n \mu_{\rm s}^n\right), \\ \phi(\mu_{\rm a}, \mu_{\rm s}, n) &= \left(c_0 + c_1 \mu_{\rm a}^1 + \cdots + c_n \mu_{\rm a}^n\right) \\ &\quad \times \left(d_0 + d_1 \mu_{\rm s}^1 + \cdots + d_n \mu_{\rm s}^n\right). \end{aligned} \quad (3)$$

Simulations (results not shown here) show that $n = 5$ is enough to gain results with acceptable accuracy.

The initial guesses of the optical properties in the following reconstruction are $\mu_{\rm a} = 0.3$ $\rm cm^{-1}$ and $\mu_{\rm s} = 60$ $\rm cm^{-1}$. Iteration is stopped until the sum of the square difference is minimized and the optical properties at that step are assigned as the "true" optical properties of the target.

Figure 3 shows the comparison between the reconstructed results by using FT and Eq. (1). Eight groups of data are reconstructed. The optical properties are the typical values of normal and cancerous cervical tissue. $\mu_{\rm a}$ of groups 1 to 8 is from 0.15 to 0.5 $\rm cm^{-1}$ with an increment of 0.05 $\rm cm^{-1}$. $\mu_{\rm s}$ of groups 1 to 8 is from 30 to 100 $\rm cm^{-1}$ with an increment of 10 $\rm cm^{-1}$. It can be seen that with the fast calculation illustrated in Eq. (1), the relative error in reconstruction is less than that with FT.

To demonstrate the performance of the technique in reconstructing optical properties, reconstruction for only one (the other is assumed known) or both of $\mu_{\rm a}$ and $\mu_{\rm s}$ are conducted.

Figure 4(a) shows the reconstructed $\mu_{\rm a}$ when $\mu_{\rm s}$ is fixed to 60 $\rm cm^{-1}$. It is shown that the relative errors are less

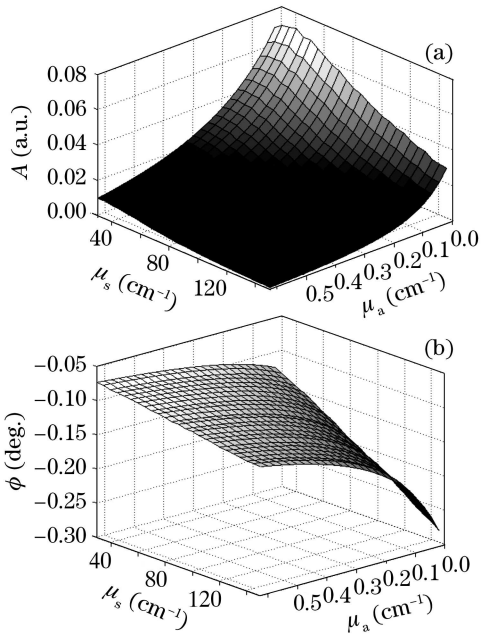


Fig. 2. Changes in (a) amplitude $A$ and (b) phase $\phi$ with the optical properties $\mu_{\rm a}$ and $\mu_{\rm s}$.

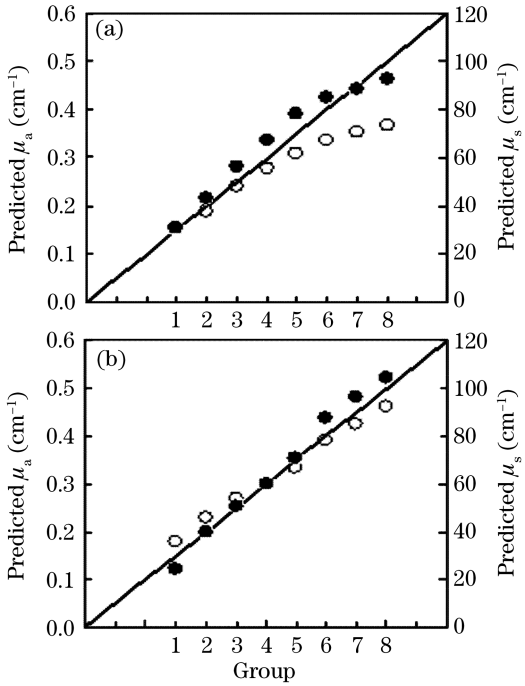


Fig. 3. Reconstructed results by using (a) FT and (b) Eq. (1). Circles represent $\mu_{\rm a}$, dots are $\mu_{\rm s}$.

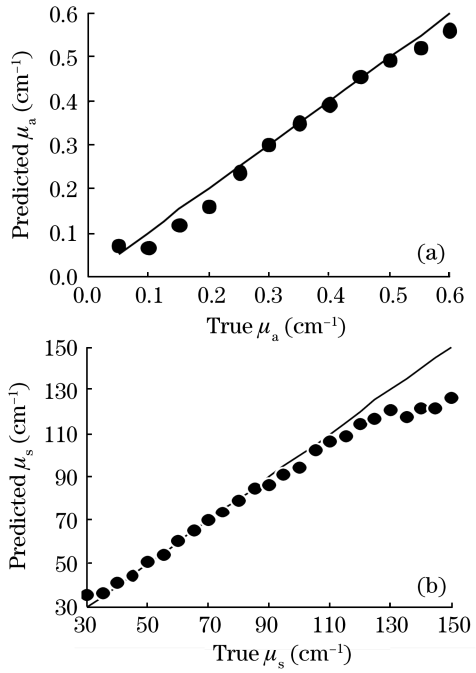


Fig. 4. Reconstructed $\mu_a$ and $\mu_s$ for the case that one of the optical properties is fixed. (a) Reconstructed $\mu_a$ for $\mu_s = 60$ cm$^{-1}$; (b) reconstructed $\mu_s$ for $\mu_a = 0.3$ cm$^{-1}$.

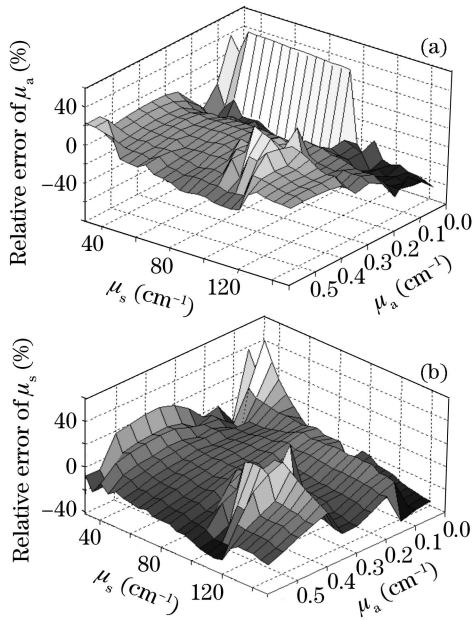


Fig. 5. Relative errors in reconstruction of (a) $\mu_a$ and (b) $\mu_s$ when the two parameters are unknown.

than ±6% in the range of $\mu_a = 0.25 - 0.6$ cm$^{-1}$ but turn to be large while $\mu_a < 0.25$ cm$^{-1}$. Figure 4(b) shows the reconstructed $\mu_s$ while $\mu_a$ is fixed to 0.3 cm$^{-1}$. It can be seen that the relative errors are less than ±6% in the range of $\mu_s = 35 - 90$ cm$^{-1}$ and turn to be large while $\mu_s > 90$ cm$^{-1}$.

Figures 5(a) and (b) show the reconstruction results of $\mu_a$ and $\mu_s$, respectively, when both of them are unknown. The accuracy of the reconstruction is similar to that in Fig. 4. For the optical properties of normal cervical tissue, the relative error can be less than ±6%. For optical properties of precancerous lesions, the relative error can be expected to be less than ±10%. The error turns to be large in the regions with small ($< 0.1$ cm$^{-1}$) or big ($> 0.5$ cm$^{-1}$) $\mu_a$. The applicability of the developed algorithm for large scale of optical properties will be investigated in the future.

In conclusion, a fast inverse MC method is presented in this letter. For all the test cases, it needs less than 1 min to complete the extraction of one set of $\mu_a$ and $\mu_s$. The results also demonstrate that the relative reconstruction errors with the developed method are less than ±10% for the optical properties of the normal cervical tissue and precancerous lesions. The inversion scheme developed in this letter is also applicable to arbitrary geometric configurations and down to length scales that approach the single-scattering mean free path.

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