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The Use of the Monte Carlo Method to Determine Optical Parameters of Tissue

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The paper presents the use of the Monte Carlo method to determine the optical parameters of tissue from steady-state diffuse reflectance measurements.

Key words: optical parameters, Monte Carlo simulation, effective attenuation coefficient, reflectance measurements.

Introduction

Optical properties of biological tissues are of great importance in optical techniques used in medical diagnosis [1, 2, 3, 4, 5]. The measurements of optical properties quickly and relatively cheaply pose a serious challenge [6, 7, 8]. Steady-state diffuse reflectance measurements make it possible to determine the effective attenuation coefficient [6, 7, 8]. What is required is to fit an assumed light propagation model to the measured values of light intensity. The aim of this work was to develop a fast and simple method of effective attenuation coefficient *in vivo* measurements using the Monte Carlo simulation, which represents the most accurate model of light propagation in turbid tissues.

Theory and Modelling

In this section we shall describe two models of radiation transport used to determine the effective attenuation coefficient from spatially resolved measurements of diffuse reflectance. The first one is a Monte Carlo simulation of photon transport that involves no physical approximations. The second approach uses an approximate transport model to generate an analytic expression for the spatially resolved reflectance. A diffusion model was used to generate analytical expressions for the reflectance.

In a radiation transport problem, the Monte Carlo method involves recording photon histories as they are scattered and absorbed. This method is attractive because it can be easily implemented and sufficiently flexible so that complex tissues may be modeled. Theoretically, the Monte Carlo solutions can be obtained to any desired accuracy. However, the accuracy is proportional to $\frac{1}{\sqrt{N}}$ where N is the number of photons propagated.

Figure 1 shows a flowchart for the photon tracing part of the Monte Carlo calculation, used in the Borland C++ Builder programme. At the start of the simulation a new photon is launched by being injected into the tissue at the origin. The starting direction of the photon movement is orthogonal to the tissue boundary, and the photon weight is taken to be 1. A variable step size method was used, in which distance Δs , at which the photon interacts with tissue, is sampled from the exponential distribution:

$$\Delta s = -\frac{\ln \xi}{\mu_a + \mu_s}$$

where ξ is a random variable with uniform distribution over the range (0, 1), μ_a is an absorption coefficient [cm^{-1}], and μ_s is the scattering coefficient [cm^{-1}]. Then, distance Δs is compared with the distance to the boundary d_b . If Δs is greater than d_b , the photon with coordinates (x, y, z) is moved into a new position (x', y', z')

$$\begin{aligned} x' &= x + \Delta s \cdot \mu_x \\ y' &= y + \Delta s \cdot \mu_y \\ z' &= z + \Delta s \cdot \mu_z \end{aligned}$$

where μ_x, μ_y, μ_z are directional cosines. Next, absorption and scattering are calculated.

Figure 1. A flowchart for tracing photons in the Monte Carlo simulation.

Once the photon has reached an interaction site, the fraction of the photon weight ΔW , absorbed by the tissue, must be calculated

$$\Delta W = \frac{\mu_a}{\mu_a + \mu_s} W$$

This weight fraction which is deposited in a local grid element and the photon weight is decreased by ΔW

$$W' = W - \Delta W$$

The calculation of the scattering involves determination of a new photon movement direction, using the Henyey-Greenstein probability distribution [3] of cosine of the deflection angle $\cos \theta$

$$p(\cos \theta) = \frac{1 - g^2}{2(1 + g^2 - 2g \cos \theta)^{3/2}} W$$

where g is an anisotropy coefficient.

The choice of $\cos \theta$ can be expressed as a function of the random variable ξ , uniformly distributed over the interval $(0, 1)$

$$\cos \theta = \begin{cases} 2\xi - 1 & \text{if } g = 0 \\ \frac{1}{2g} \left[1 + g^2 - \left(\frac{1 - g^2}{1 - g + 2g\xi} \right)^2 \right] & \text{if } g \neq 0 \end{cases}$$

Next, the azimuthal angle φ , which is uniformly distributed over the interval $(0, 2\pi)$, is sampled

$$\varphi = 2 \pi \xi$$

where variable ξ is uniformly distributed over the interval $(0, 1)$.

Then, the new direction of the photon (μ'_x, μ'_y, μ'_z) can be calculated

$$\begin{aligned} \mu'_x &= \frac{\sin \theta}{\sqrt{1 - \mu_z^2}} (\mu_x \mu_y \cos \varphi - \mu_y \sin \theta) + \mu_x \cos \theta \\ \mu'_y &= \frac{\sin \theta}{\sqrt{1 - \mu_z^2}} (\mu_y \mu_z \cos \varphi + \mu_x \sin \theta) + \mu_y \cos \theta \\ \mu'_z &= -\sin \theta \cos \varphi \sqrt{1 - \mu_z^2} + \mu_z \cos \theta \end{aligned}$$

If Δ_s is not greater than d_b then the photon moves to a new position on the boundary, and the probability of it being internally reflected is computed. If the angle of the incidence is greater than the critical angle, the internal reflectance is set to 1. Otherwise, the reflectance is computed by Fresnel's formulas. The reflectance is then compared with the random variable uniformly distributed over the range $(0, 1)$. If the

variable is greater than the reflectance, then the photon is transmitted, otherwise, it is internally reflected.

Photon paths can be terminated by emission out of the tissue. For a photon still propagating inside the tissue, (provided its weight is sufficiently small after the many steps of interaction), its termination by roulette procedure is executed.

The Monte Carlo simulations were compared with an analytical model based on diffusion approximation of the radiative transport equation. For a semi-infinite medium the solution of the diffusion equation is given by [8]

$$\Phi(r, z) = \frac{I_0}{4\pi D} \cdot \left[\frac{\exp(-\mu_{eff} \sqrt{(z - z_0)^2 + r^2})}{\sqrt{(z - z_0)^2 + r^2}} - \frac{\exp(-\mu_{eff} \sqrt{(z + z_0 + 2z_b)^2 + r^2})}{\sqrt{(z + z_0 + 2z_b)^2 + r^2}} \right] \quad (1)$$

where Φ is the photon fluence rate, I_0 is the source intensity, D is the diffusion constant

$$D = \frac{1}{3(\mu_a + \mu'_s)} \quad [8], \mu'_s = (1 - g)\mu_s \text{ is the reduced scattering coefficient and } \mu_{eff} = \sqrt{\frac{\mu_a}{D}}$$

is the effective attenuation coefficient [8], $z_0 = \frac{1}{\mu'_s}$, z_b is the distance to the extrapolated

$$\text{boundary} \quad [8], \quad z_b = 2D \frac{1 + R_{eff}}{1 - R_{eff}}, \quad R_{eff} = -1.440 n_{rel}^{-2} + 0.710 n_{rel}^{-1} + 0.668 + 0.0636 n_{rel},$$

$n_{rel} = \frac{n_{tissue}}{n_{air}}$ is the relative refractive index of the tissue compared to that of air.

The values of the optical parameters estimated from a simple analytical theory can be used as the starting values for an iteration procedure in the Monte Carlo simulation fitting. To do this, we have to know the approximate value of the absorption coefficient μ_a . The reduced scattering coefficient can be computed from

$$\mu'_s = \frac{\mu_{eff}^2}{3\mu_a} - \mu_a \quad (2)$$

where μ_{eff} is the estimated value from the analytical solution.

The next step is to run two Monte Carlo simulations for two different values: μ_{eff0} , μ_{eff1} , where $\mu_{eff0} < \mu_{eff1}$, giving the light intensities $\Phi_{MC}(r, \mu'_s)$. The parameters μ_{s0} , μ_{s1} are calculated from (2). Then logarithms of the light intensity quotients are computed

$$m_{0i} = \ln \left(\frac{\Phi_{MC}(r_i, \mu'_{s0})}{\Phi_{MC}(r_0, \mu'_{s0})} \right)$$

$$m_{1i} = \ln \left(\frac{\Phi_{MC}(r_i, \mu'_{s1})}{\Phi_{MC}(r_0, \mu'_{s1})} \right)$$

$$m'_i = \frac{m_{1i} - m_{0i}}{\mu'_{s1} - \mu''_{s1}}$$

The total approximation error is obtained from (3) as the function of the optical parameter's increase $\Delta\mu'_s$

$$E(\Delta\mu'_s) = \sum_{i=1}^n (m_{0i} + m'_i \Delta\mu'_s - y_i)^2 \quad (3)$$

The function $E(\Delta\mu'_s)$ has a minimum for the condition

$$\frac{dE}{d\Delta\mu'_s} = 0$$

The derivative being

$$\begin{aligned} \frac{dE}{d\Delta\mu'_s} &= 2 \sum_{i=1}^n (m_{0i} + m'_i \Delta\mu'_s - y_i) m'_i \\ \frac{dE}{d\Delta\mu'_s} &= 2 \sum_{i=1}^n (m_{0i} - y_i) m'_i + 2 \Delta\mu'_s \sum_{i=1}^n m'^2_i \end{aligned}$$

The value of the optical parameter's increase, which minimizes the total error is

$$\Delta\mu'_s = \frac{\sum_{i=1}^n (m_{0i} - y_i)}{\sum_{i=1}^n m'^2_i} \quad (4)$$

The improved value of $\Delta\mu'_s$ is

$$\mu'_s = \mu'_{s0} + \Delta\mu'_s \quad (5)$$

The value of μ_{eff} is

$$\mu_{\text{eff}} = \sqrt{3\mu_a(\mu_a + \Delta\mu'_s)} \quad (6)$$

The variance of $\Delta\mu'_s$ is

$$\text{var}(\mu'_s) = \text{var}(\Delta\mu'_s) = \sum_{i=1}^n \left| \frac{\partial \Delta\mu'_s}{\partial y_i} \right|^2 \sigma^2(y_i)$$

The variance of μ_{eff} is

$$\text{var}(\mu_{\text{eff}}) = \left| \frac{\partial \mu_{\text{eff}}}{\partial \mu'_s} \right|^2 \text{var}(\mu'_s) = \left(\frac{3\mu_a}{2\mu_{\text{eff}}} \right)^2 \text{var}(\mu'_s) \quad (7)$$

If we assume that the main source of the uncertainty of the measured photon fluence rate Φ is a random optical contact of the detector with tissue [9], then the standard deviation of the measured value of Φ is proportional to Φ with the coefficient α

$$\sigma(\Phi) = \alpha\Phi$$

The variance $\text{var}(y_j)$ is expressed by the variance of the measured photon fluence rate and is given by

$$\text{var}(y_i) = \frac{\text{var}(\Phi_i)}{\Phi_i^2} = \alpha^2$$

Then we can calculate the variance of μ_{eff} as

$$\text{var}(\mu_{\text{eff}}) = \alpha^2 \left(\frac{3\mu_a}{2\mu_{\text{eff}}} \right)^2 \frac{n}{\left(\sum_{i=1}^n m_i'^2 \right)^2} \quad (8)$$

The equations given above were used to estimate the measuring error.

Materials and Methods

The surface light intensity distributions were measured for a human forearm *in vivo* by means of sophisticated one-channel microprocessor system [9]. The system, described elsewhere [9], consists of a light detector (silicon photodiode), a switched integrator and a microprocessor with a built-in 10-bit analogue-to-digital converter. The tissue under examination was coupled with the light detector by fiber optics. The device was controlled by a personal computer via a serial RS232 interface. The light source was an LED emitting light wavelength of about 660 nm [9]. The Monte Carlo programme, called MC_TEST, was written in C++. The programme was used to simulate light propagation in turbid tissues.

Results

The results of measurements were processed by the method proposed in [8]. The approximate values of the effective attenuation coefficient were determined. These values served as the starting points for an iteration procedure (5). The value of 0.3 cm^{-1} was adopted for the absorption coefficient for the human tissue [7]. The approximate values of the reduced scattering coefficient $\Delta\mu'_s$ were calculated from equation (2). Two Monte Carlo simulations were made: the first one for the calculated value of $\Delta\mu'_s$, and the second one for the value of $\Delta\mu'_s$ increased by 1 cm^{-1} . Then the improved values of $\Delta\mu'_s$ as well as the improved values of the effective attenuation coefficient were computed from (5) and (6), respectively.

The results of the determination of the effective attenuation coefficient for the human forearm tissue *in vivo* are shown in Table 1.

Table 1. Results of the determination of the effective attenuation coefficient.

Person	Forearm	μ_{eff} from the Monte Carlo [cm^{-1}]
A	Left	2.10 ± 0.23
A	Right	2.32 ± 0.29
B	Left	2.63 ± 0.20
B	Right	2.53 ± 0.20

Person	Forearm	μ_{eff} from the Monte Carlo [cm^{-1}]
C	Left	2.49 ± 0.27
C	Right	2.31 ± 0.27
D	Left	2.70 ± 0.22
D	Right	2.51 ± 0.27
E	Right	2.18 ± 0.29

Comparison of the Monte Carlo with the diffusion theory is shown in figure 2.

Figure 2. Comparison of the Monte Carlo with the diffusion theory.

The correlation coefficient was found to be 0.9932 for the significance level of less than 0.000001. The computed values are slightly greater than those estimated from the simple diffusion model [9]. The range of the estimated values of the effective attenuation coefficient ranged between 2 cm^{-1} and 3 cm^{-1} . These results are compatible with those given in [6, 7, 8].

Discussion and Conclusions

Our method is simple, fast and inexpensive. It makes it possible to find the effective attenuation coefficient from light intensity measurements for a few places on the tissue examined. The results obtained by the Monte Carlo method are in good agreement with those obtained from a simple analytical theory [9]. The Monte Carlo simulation is a very useful method to fit the results of measurements to the complete physical model.

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