Inverse Algorithm Optimization for Determining Optical Properties of Biological Materials from Spatially-resolved Diffuse Reflectance

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INTRODUCTION

Optical characterization of biological materials using an inverse radiation transport approach is useful in biomedical diagnosis and nondestructive quality evaluation of food and agricultural products. However, accurate determination of the optical properties from intact biological materials based on light transport theory is challenging because of the complex mathematical model and sophisticated instrumentation and experimental procedure.

Different approaches and methods have been developed for determining the optical properties of turbid media. In this work, a diffusion theory model for spatially-resolved steady-state reflectance was chosen because it provides accurate description of radiation transport in turbid media, needs less computational time, and is particularly useful for nondestructive measurement.

The optical parameter estimation was formulated as a nonlinear least squares optimization problem based on several important assumptions (i.e., constant variance errors, uncorrelated errors, and the Gaussian distribution of errors). Proper data transformation and weighting methods should be considered when some of the assumptions are violated. Moreover, to improve the accuracy of the parameter estimation, the inverse algorithm needs to be optimized and the information involving model efficiency, curve fitting errors, and parameter characteristics should be acquired and analyzed.

OBJECTIVES

- Examine different data transformation and weighting methods for nonlinear least squares estimates;
- Perform sensitivity analysis to determine an appropriate data transformation/weighting method to improve the inverse algorithm;
- Assess the robustness of the diffusion model and the inverse algorithm using statistical analysis.

FORWARD PROBLEM

Diffusion Model

Light transfer in a medium is governed by the radiation transport theory. For most biological materials in which light scattering is dominant, diffusion approximation to the radiation transport equation is valid. The diffuse reflectance at the surface of the turbid medium (R) as a function of the source-detector distance (r) as well as two unknown optical parameters (μ_a & μ_s') of the medium is given by

$$R(r)=\frac{C_1}{4\pi D}\left[\frac{\exp(-\mu_{eff}r_1)}{r_1}-\frac{\exp(-\mu_{eff}r_2)}{r_2}\right]+\frac{C_2}{4\pi}\left[z_0(\mu_{eff}+\frac{1}{r_1})\frac{\exp(-\mu_{eff}r_1)}{r_1^2}+(z_0+2z_b)(\mu_{eff}+\frac{1}{r_2})\frac{\exp(-\mu_{eff}r_2)}{r_2^2}\right]$$

where μ_a and μ_s' are absorption and reduced scattering coefficients, respectively.

Monte Carlo Simulation

For accurate estimation of the optical parameters of turbid media, the diffusion model and inverse algorithm were validated by Monte Carlo (MC) simulations. Figure 1 illustrates the MC simulation for estimating diffuse reflectance and internal photon absorption in a turbid medium.

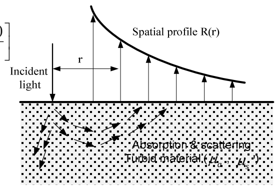

Fig. 1. Monte Carlo simulation for diffuse reflectance and internal photon absorption in a turbid medium.

INVERSE PROBLEM

Nonlinear Least Squares Inverse Algorithm

Nonlinear least squares method was used to find the minimum of the sum of squares of the difference between the true reflectance and predicted reflectance values with estimated parameters. A large-scale algorithm such as a subspace trust-region method based on the interior-reflective Newton approach was selected to achieve the algorithm optimization.

Data Transformation and Weighting Methods

Logarithm-transformed diffusion model (LTDM): $R_{\log}(r)=\log\left[R(r)\right]$

Integral-transformed diffusion model (ITDM): $R_{\text{int}}(r)=\int_0^r R(\rho)\rho\, d\rho$

Diffusion model with relative weighting (RWDM): $\sum\left[(R_{obs}-R_{pred})/R_{obs}\right]^2$

Sensitivity Analysis

Sensitivity coefficients of original diffusion model (ODM), LTDM, ITDM, and RWDM are calculated by

$X_{ori\_\beta}=\beta\frac{\partial R}{\partial\beta}$ $X_{\log\_\beta}=\beta\frac{\partial\log(R)}{\partial\beta}$ $X_{\text{int}\_\beta}=\beta\frac{\partial R_{\text{int}}}{\partial\beta}$ $X_{RW\_\beta}=\beta\frac{\partial R}{R\partial\beta}$ where β represents optical parameters μ_a and μ_s'.

SIMULATION EXPERIMENTS

To validate the diffusion model and the inverse algorithm using MC simulations, the medium was considered to be turbid and semi-infinite. MC simulations were performed with the absorption and reduced scattering coefficients as two input parameters, which determine the simulation results.

Thirty-six different combinations of μ_a and μ_s' were selected, which span a large range of values: $0.004<\mu_a<0.800$ mm^{-1}, $0.40<\mu_s'<4.00$ mm^{-1}, and $5<\mu_s'/\mu_a<100$. These values were chosen based on the published data for the optical properties of fruit and other food products. The refractive index of the medium was assumed to be 1.35, similar to that of fruit. A total of 3×10^6 photons and 0.1 mm spatial resolution of both radial distance and depth were used to produce the reflectance for the spatial distance of 0.1- 10 mm. The MC generated diffuse reflectance profiles were then fitted by the inverse algorithm for the diffusion model to deduce the optical properties of the media.

RESULTS

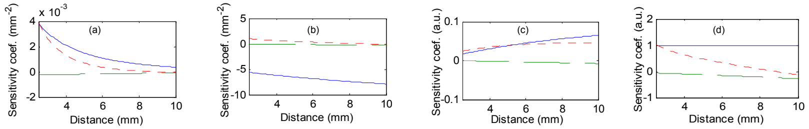

Fig. 2. Sensitivity coefficients of the optical parameters (μ_a =0.006 mm^{-1} & μ_s'=0.40 mm^{-1}) as functions of the source-detector distance for ODM, LTDM, ITDM, and RWDM. Solid curves stand for R, dash curves for μ_a and dot curves for μ_s'.

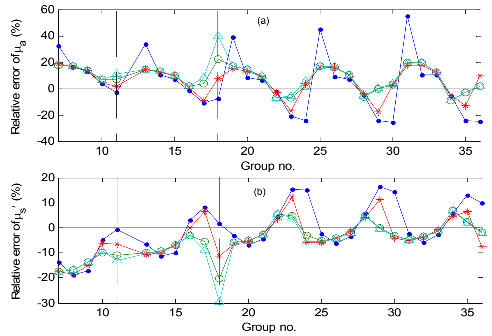

Fig. 3. Relative errors of estimating 29 groups of (a) μ_a and (b) μ_s' by the original model, and the three data transformation and relative weighting methods: ODM (●), LTDM (○), ITDM (✳), RWDM (△).

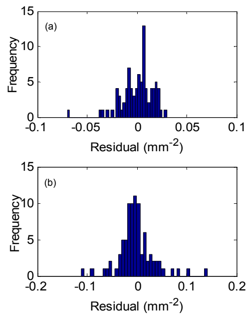

Fig. 4. Residual histograms for the reflectance data from LTDM with (a) μ_a =0.006 mm^{-1} & μ_s'=0.40 mm^{-1}, and (b) μ_a =0.057 mm^{-1} & μ_s'=4.00 mm^{-1}.

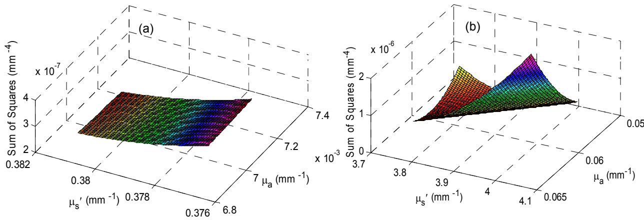

Fig. 5. 3-D plot of sum of squares for (a) group 25 with μ_a =0.006 mm^{-1} & μ_s'=0.40 mm^{-1}, and (b) group 30 with μ_a =0.057 mm^{-1} & μ_s'=4.00 mm^{-1} using the LTDM method.

Table 1. Statistical results for estimating the optical parameters using the logarithm-transformed diffusion model (LTDM).

Group no.	parameter	True value (mm^{-1})	Estimated value (mm^{-1})	Standard Error (mm^{-1})	Relative Error (%)	95% asymptotic confidence interval
25	μ_a	0.006	0.007	0.0015	16.7	[0.0069, 0.0072]
	μ_s'	0.40	0.38	0.023	-5.0	[0.377, 0.381]
30	μ_a	0.057	0.059	0.0129	3.5	[0.0560, 0.0616]
	μ_s'	4.00	3.88	0.660	-3.0	[3.734, 4.002]

CONCLUSIONS

- Sensitivity analysis demonstrates that the reduced scattering coefficient can be estimated more accurately than the absorption coefficient, which is validated by Monte Carlo simulation results.
- The logarithm and integral transformation of the original data and the relative weighting method greatly improve the estimations of the two optical parameters with the relative errors of 10.4%, 10.7%, and 11.4% for μ_a, and 6.6%, 7.0% and 7.1% for μ_s'.
- Further statistical analysis shows that the logarithm transformation and relative weighting methods can improve the inverse algorithm to obtain more reliable estimations of the two optical parameters.

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