Modeling and reconstruction of diffuse optical tomography using adjoint method

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SUMMARY

A new finite-element algorithm based on adjoint method is developed to solve the inverse problem of frequent-domain diffusion equation for soft tissues. With the analytical form of gradients, the adjoint method is expanded to complex domains for the reconstruction of optical parameters in diffuse optical tomography accurately and efficiently. Specific numerical simulations are carried out and compared to validate the proposed algorithm. The results demonstrate that the algorithm is stable and robust to reconstruct optical parameters. Copyright © 2008 John Wiley & Sons, Ltd.

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1. INTRODUCTION

Diffuse optical tomography (DOT), an emerging optical imaging technique, uses arrays of sources and detectors to obtain spatially dependent optical parameters of the tissue. The concept of DOT is to reconstruct the optical properties of tissues to detect physiological changes by recognizing changes in the optical parameters of scattering and absorption of various biological tissues. Many efforts have been made to develop algorithms to solve this inverse problem. Arridge et al. [1] and Boas et al. [2] developed analytical modeling techniques for simple homogeneous objects or media with a single spherical perturbation. Statistical modeling techniques (Monte Carlo method [3–5])
and random walk theory [6–9] have also been developed. While these methods offer flexibility in modeling complex geometries with derived parameter distributions and individual photon histories, they require very lengthy computational time [10]. Recently, a numerical technique based on finite-element method (FEM) has been widely used for DOT parameter reconstruction, introduced by Arridge et al. [11–14]. The optical properties distribution is reconstructed by an iterative procedure that involves solving the forward problem a number of times and updating the optical properties to fit experimental measurements. Because the inverse problem in DOT is a non-unique, ill-posed underdetermined problem, developing an efficient and robust reconstruction algorithm is still a challenge.

In this paper a new algorithm based on larger-scale limit-memory Broyden–Fletcher–Goldfarb–Shanno (BFGS) adjoint method is described. The original BFGS (L-BFGS) optimization method, developed by Liu and Nocedal [15], requires accurate, user-supplied gradients of the objective functions. To date, most algorithms rely on certain forms of Newton iteration, which include the Jacobian-matrix calculation with a great computational cost, since forming the matrix is equivalent to solving forward problem many times [16]. The adjoint method provides a new means to compute the accurate gradients analytically and save the computational cost significantly [17]. Oberai et al. [18] introduced the adjoint method to isotropic elastography and Liu et al. [19] developed the algorithm for general anisotropic cases. The objective of this study is to expand the BFGS adjoint method to complex domain so that the frequency-domain diffusion equation in DOT can effectively be solved. A phantom experiment is carried out by a multifrequency near-infrared DOT system. A finite-element model is set up to simulate the experiment and optical parameters are reconstructed by measurement. Comparisons between experiment and simulation data are conducted to validate the proposed algorithm.

The paper is organized as follows. In Section 2, a finite-element optimization-based algorithm is derived to solve the inverse problem of diffusion equation in the frequency domain. A phantom experiment is described in Section 3. Our numerical model is given in Section 4, followed by our results, discussion and conclusions.

2. METHODOLOGY

Under the assumption that light scattering dominates absorption in a medium, the transport of a photon in a tissue can be described by a diffusion equation. In the frequency domain, it is expressed as

$$-\nabla \cdot D(x) \nabla \Phi(x, \omega) + \mu_a \Phi(x, \omega) + \frac{i \omega}{c} \Phi(x, \omega) = S(x, \omega)$$

with the Robin boundary condition

$$\Phi + 2DA \hat{n} \cdot \nabla \Phi = 0$$

where $S(x, \omega)$ is an isotropic light source at position $x$, $\omega$ the frequency of light source, $\Phi(x, \omega)$ the photon density at $x$, $c$ the speed of light in the tissue, $\mu_a$ the absorption coefficient, $D = 1/(3(\mu_a + \mu'_s))$ the diffusion coefficient, $\mu'_s$ the reduced scattering coefficient, $A = (1 + \gamma)/(1 - \gamma)$ and $\gamma$ is the parameter governing the internal reflection at the boundary. After finite-element
where the adjoint

\[
[K_R]\{\phi_R\} - [K_I]\{\phi_I\} = \{S\}
\]

where ‘R’ represents the real part and ‘I’ the imaginary part.

where \( \{w\} \) is calculated via

\[
\begin{align*}
\delta G &= \{w_R\}^T[\delta K_R]\{\phi_R\} - \{w_I\}^T[\delta K_I]\{\phi_I\} \\
&= \{(\phi_R) - \{\phi_R^m\}\}^T[X_R][(\phi_R) - \{\phi_R^m\}] + \{(\phi_I) - \{\phi_I^m\}\}^T[X_I][(\phi_I) - \{\phi_I^m\}] \\
&= \text{minimal once } \{\phi\} \text{ is solved (Equation (3))}.
\end{align*}
\]

The details to derive the adjoint \( \{w\} \) and the gradient \( G \) are given in the Appendix.

It is noted that \( \{\phi\} \) and \( \{w\} \) share the same Cholesky factorization [20] for \( [K] \); thus, the computational expense for solving \( \{w\} \) (Equation (6)) is minimal once \( \{\phi\} \) is solved (Equation (3)). At the same time, once adjoint \( \{w\} \) is calculated, gradients for different parameters are calculated by Equation (5), which share the adjoint field. The feature makes the adjoint method not impacted by the number of unknown parameters significantly. The iterative optimization procedure is shown in Figure 1.

3. EXPERIMENT

The experimental testing was conducted with the frequency-domain DOT system developed at the Center for Functional Onco-Imaging, UC-Irvine. The DOT system is based on a network analyzer that not only measures the amplitude and the phase of the detected signals, but also provides RF signals to modulate the amplitude of laser diode sources. The details of the system were given in Gulsen et al. [21]. While the system employs four different wavelengths, only the data acquired at 785 nm were used in this study. Photomultiplier tubes were used as detectors to measure low-level signals in fan-beam geometry. Optical fibers were used both to conduct light from the sources to the tissue and to transfer the collected light from the tissue to the detectors. The 62.5 μm core diameter gradient-index fibers were used as the source fibers, while the 1.1 mm core diameter step-index fibers were used as the detector fibers. An adaptive interface was constructed to hold the sample and position the tips of source and detector fibers around the full circumference of the sample. The interface consists of eight-source and eight-detector fiber probes with radically adjustable holders. The phantoms were placed at the center of the fiber optic interface and the fiber probes adjusted radically until they contacted the sample.
Measured source \( S \)

Finite-element mesh for phantom

Measured light intensity \( \phi_m \)

Initial estimate for distribution of (\( \mu_a, \mu'_s \))

Solve Eq. (3) for light intensity \( \phi \)

Compare: \( \phi - \phi_m \)

Calculate objective function \( G \) Eq. (4)

Evaluate \( G \) small enough?

Yes

Output(\( \mu_a, \mu'_s \))

No

Solve Eq. (6) for adjoint field \( w \)

Calculate gradients \( \partial G / \partial \mu_a, \partial G / \partial \mu'_s \)

L-BFGS Optimization: update (\( \mu_a, \mu'_s \)) with

\( G, \partial G / \partial \mu_a, \partial G / \partial \mu'_s \)

Figure 1. Flowchart of DOT reconstruction of optical coefficients in frequent domain.

Two 63-mm-diameter solid phantoms simulating tissue optical properties were used in the experiment. The optical properties of phantoms are \( \mu_a = 0.0132 \text{mm}^{-1} \) and \( \mu'_s = 0.86 \text{mm}^{-1} \) at 785 nm. One was used for calibration purposes (homogeneous case). A 15-mm hole was drilled into the second phantom to simulate different embedded objects (heterogeneous case). The hole was positioned halfway between the center and the edge and was filled with a mixture of Intralipid and Indian ink in water to simulate a higher absorbance object with \( \mu_a = 0.0264 \text{mm}^{-1} \). The homogeneous phantom calibration measurement was performed to account for and calibrate the fiber differences in transmission and alignment and the discretization errors due to data and model mismatch [22]. After calibration, the absorption and scattering maps were reconstructed using the inverse solver. Sixty-four amplitude and phase data at 785 nm are given and converted to the real and imaginary parts to compare with numerical results.

4. NUMERICAL MODEL

Based on the phantom and experimental systems, we established a 2-D FEM consisting of a circle matrix with an embedded inclusion (thick mesh) (Figure 2). The eight solid circles represent the detectors, while the eight open circles represent the light sources. The sources and detectors are placed uniformly on the external surface with 45° apart. The model is discretized with standard 2-D triangle elements having 3264 elements and 1761 nodes. A constant light source is applied and the intensities on surface are then detected. The difference between calculated and measured values is employed to reconstruct optical coefficients. It is noted that, although the light sources are placed on the phantom surface, the diffusion equation cannot describe the collimated source correctly. A common approach to overcome this limitation is to represent a collimated pencil beam by an isotropic point source located at a depth \( 1/\mu'_s \) below the tissue surface [10]. Using this approach, the eight light-source locations were calculated.
5. RESULTS AND DISCUSSION

Once an initial estimation of optical coefficients ($\mu_a$ and $\mu'_a$) is obtained, the light intensity distribution can be calculated by using Equation (3). Calculations of the optical coefficients can be optimized by comparing the calculated and measured values at key points. Stable reconstructed coefficients were generated, regardless of the initial estimates. The convergent curves for optical parameters are plotted in Figure 3, which demonstrates that values for the $\mu_a$ and $\mu'_a$ of the matrix approach the measured value rapidly. After approximately 30 iterations, the relative errors are within the range of 5%. Then they exhibit some minor adjustment. In contrast, coefficients of inclusion converge slower. They begin to approach the real values after 45 interactions and reach the true values after 55 steps, with a maximum error of 18%.

The real and reconstructed optical coefficients are listed in Table I, which indicates that parameters for the matrix are reconstructed more accurately, with an error of less than 1%, while the reconstructed parameters of the inclusion have a relative error of about 15%.

The slower convergence and coarse accuracy of parameters for the inclusion are explained by their influence on the surface measurements. In general, parameters having a significant influence on the surface measurement are also those that are most accurately and easily identified. The convergent curves demonstrate that coefficients for the inclusion do not have as significant an impact on the surface measurements as do those of the phantom matrix.

Previous DOT studies frequently face the problem of the low resolution of reconstructed images [23]. Prior structural information has been applied to improve the resolution [24]. In our
Figure 3. Convergent curves for optical parameters.

Table I. Real and reconstructed optical coefficients.

<table>
<thead>
<tr>
<th>Matrix</th>
<th>Inclusion</th>
</tr>
</thead>
<tbody>
<tr>
<td>μ_a</td>
<td>μ'_a</td>
</tr>
<tr>
<td>μ'_s</td>
<td>μ_s</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Real values</th>
<th>Reconstruction</th>
</tr>
</thead>
<tbody>
<tr>
<td>μ_a</td>
<td>0.0132</td>
<td>0.0132</td>
</tr>
<tr>
<td>μ'_s</td>
<td>0.8582</td>
<td>0.8580</td>
</tr>
<tr>
<td>μ_a</td>
<td>0.0264</td>
<td>0.0240</td>
</tr>
<tr>
<td>μ'_s</td>
<td>0.8582</td>
<td>0.720</td>
</tr>
</tbody>
</table>

study, the location of inclusion is assumed to be obtained by MRI or CT. With prior structural knowledge, only four optical parameters are needed to be reconstructed, which makes it possible to decrease the errors of optical parameters significantly. It is found that the largest error is 15% in our study, while the error can be 30% without prior information [24]. Furthermore, an advantage of our adjoint method is to save the computational cost. Once the adjoint field \( \{ w \} \) is calculated, the gradient of objective function can be obtained by using Equation (5) directly. Different unknown parameters share the same adjoint field \( \{ w \} \), which saves the computational cost significantly during iterations. This unique feature of the adjoint method can widen its application in different reconstruction algorithms.

6. CONCLUSIONS

We developed a new finite-element algorithm based on BFGS adjoint method to solve the inverse problem of the frequency-domain DOT diffusion equation. The proposed adjoint method provides a new means to compute the gradients of objective function analytically. Significant computational saving is realized by utilizing the solution of adjoint equation. We expand this method to complex...
domains to compute the gradients in DOT. By comparing measurements derived from phantom experiments with numerical simulations, we found our algorithm to be stable and robust for reconstructing the optical parameters. These results are sufficiently encouraging to warrant further development and future clinical evaluation of this adjoint method for DOT reconstruction.

APPENDIX A

The diffusion equation (Equation (1)) and boundary condition (Equation (2)) can be rewritten as

\[ \text{the FEM form (Equation (3)) with the objective function shown in Equation (4). The discretized FEM weak form can be further obtained as} \]

\[ \{w_R\}^T([K_R]\{\phi_R\} - [K_1]\{\phi_1\} - \{S\}) = 0 \]

\[ -\{w_1\}^T([K_R]\{\phi_1\} + [K_1]\{\phi_R\}) = 0 \]  \hfill (A1)

where \{w\} is the adjoint field.

The Lagrangian is consequently discretized as

\[ L(\mu_a, \mu_s', \{\phi\}, \{w\}) = ((\phi_R) - (\phi^m_R))^T[K_R](\phi_R) - (\phi^m_R)) + ((\phi_1) - (\phi^m_1))^T[X_1](\phi_1) - (\phi^m_1)) \]

\[ + (w_R)^T([K_R]\{\phi_R\} - [K_1]\{\phi_1\} - \{S\}) - (w_1)^T([K_R]\{\phi_1\} + [K_1]\{\phi_R\}) \] \hfill (A2)

It is shown that \( G(\mu_a, \mu_s') = L(\mu_a, \mu_s', \{\phi\}, \{w\}) \) and \( \delta G = \delta L \) as Equation (A1) is satisfied for arbitrary \{w\}. Then \( \delta L \) can be expressed as

\[ \delta L = 2((\phi_R) - (\phi^m_R))^T[X_R] + (w_R)^T[K_R] - (w_1)^T[K_1]\delta \phi_R \]

\[ + 2((\phi_1) - (\phi^m_1))^T[X_1] - (w_R)^T[K_1] - (w_1)^T[K_R]\delta \phi_1 \]

\[ + (w_R)^T([\delta K_R]\{\phi_R\} - [\delta K_1]\{\phi_1\}) - (w_1)^T([\delta K_R]\{\phi_1\} + [\delta K_1]\{\phi_R\}) \] \hfill (A3)

In order to compute \{w\}, let

\[ 2((\phi_R) - (\phi^m_R))^T[X_R] + (w_R)^T[K_R] - (w_1)^T[K_1] = 0 \] \hfill (A4)

and

\[ 2((\phi_1) - (\phi^m_1))^T[X_1] - (w_R)^T[K_1] - (w_1)^T[K_R] = 0 \] \hfill (A5)

Equations (A4) and (A5) can then be rewritten as

\[ [K_R]\{w_R\} - [K_1]\{w_1\} = -2[X_R](\{\phi_R\} - (\phi^m_R)) \] \hfill (A6)

and

\[ [K_R]\{w_1\} + [K_1]\{w_R\} = 2[X_1](\{\phi_1\} - (\phi^m_1)) \] \hfill (A7)

Combining Equations (A6) and (A7), we can obtain

\[ ([K_R] + i[K_1])(\{w_R\} + i\{w_1\}) = -2[X_R](\{\phi_R\} - (\phi^m_R)) + i2[X_1](\{\phi_1\} - (\phi^m_1)) \]  \hfill (A8)
\[
[K][w] = -2[X_R](\{\phi_R\} - \{\phi_R^m\}) + i2[X_I](\{\phi_I\} - \{\phi_I^m\}) \tag{A9}
\]

It is noted that the matrix \([K]\) is as the same as that in Equation (3). Therefore, \([w]\) can be solved by using Equations (A8)–(A9) with the same method as in Equation (3).

Correspondingly,
\[
\delta G = [w_R]^T(\{\delta K_R\}[\phi_R] - [\delta K_I][\phi_I]) - [w_I]^T(\{\delta K_R\}[\phi_I] + [\delta K_I][\phi_R]) \tag{A10}
\]

Since \(K_I\) is independent with \(\mu_a\) and \(\mu'_a\), \(\delta K_I = 0, \delta G \) further reads as follows:
\[
\delta G = [w_R]^T[\delta K_R][\phi_R] - [w_I]^T[\delta K_R][\phi_I] \tag{A11}
\]

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