A Semi-smooth Newton Method for Diffuse Optical Tomography with L1-Norm and Total Variation Regularization

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Abstract. This study introduces a novel multi-measurement Diffuse Optical Tomography reconstruction method that employs both L1-norm and Total Variation regularization, solved by the semi-smooth Newton method. By integrating L1-norm regularization to address sparsity and TV regularization to preserve edges and structural details, our approach effectively combats the ill-posed nature of DOT reconstructions. The results demonstrate that our approach reduces the required iterations while simultaneously maintaining or enhancing reconstruction accuracy and robustness to noise.

Keywords: Diffuse Optical Tomography; Regularization; Radiative Transport Equation.

1. Introduction

Diffuse Optical Tomography (DOT) is an emerging biomedical optical imaging modality that reconstructs internal physiological parameters, such as oxygen saturation and blood flow, by measuring the absorption and scattering of near-infrared light by biological tissues. Compared to other imaging methods, DOT offers advantages such as being non-invasive, low-cost, and portable. It holds broad application prospects in areas including breast tumor detection, brain functional imaging, and arthritis diagnosis. However, a major challenge faced by DOT is the ill-posed nature of its image reconstruction problem. Due to the strong scattering of light by biological tissues, the light transmission process in DOT exhibits highly nonlinear and underdetermined characteristics, rendering the reconstruction problem highly sensitive to measurement noise and prior information.

To overcome this issue, researchers have proposed various regularization methods, such as Tikhonov regularization and Total Variation (TV) regularization. These methods enhance the stability and accuracy of the solution by incorporating prior information into the reconstruction process. In practical applications, DOT typically requires multiple measurements to acquire sufficient information for reconstruction. Multiple measurements not only enhance the accuracy of reconstruction but also enable dynamic imaging to monitor temporal changes in physiological parameters. However, multiple measurements also introduce challenges in terms of large data volume and high computational complexity. Therefore, efficiently solving the DOT reconstruction problem in the context of multiple measurements has become an important research topic.

This paper proposes a multi-measurement DOT reconstruction method based on L1-norm and TV regularization. L1-norm regularization effectively suppresses sparse noise in the reconstruction results, while TV regularization preserves the edges and structural information of the reconstructed images. To efficiently solve the reconstruction problem, the paper employs a semi-smooth Newton method. By introducing auxiliary variables to convert the original problem into a smooth optimization problem, and then alternately optimizing the absorption coefficients and auxiliary variables, high-quality reconstruction results can be rapidly and stably achieved. The paper provides a detailed derivation of the mathematical principles of the algorithm and validates its effectiveness through both simulations and real data. The main contributions of this paper are as follows: 1) A DOT reconstruction model employing both L1-norm and TV regularization is proposed, effectively utilizing two types of prior information: sparsity and gradient sparsity. 2) For this model, an optimization algorithm based on the semi-smooth Newton method is introduced. By incorporating auxiliary variables, the complex optimization problem is decomposed into multiple simpler subproblems for resolution. 3) Through a series of simulation and real data experiments, the
reconstruction quality and computational efficiency of the algorithm are systematically evaluated, demonstrating the superiority of the proposed algorithm over traditional methods. The structure of the rest of this paper is organized as follows: The second section reviews related work in DOT reconstruction, providing a background on existing methodologies and their limitations. The third section deduces the mathematical principles of the proposed algorithm, explaining the rationale behind the combination of L1-norm and TV regularization, as well as detailing the semi-smooth Newton method for solving the optimization problem. The fourth section presents simulation experiments to demonstrate the performance of the algorithm. This includes comparisons with traditional methods in terms of reconstruction accuracy, computational efficiency, and robustness to noise. The fifth section concludes the paper, summarizing the main findings and contributions. The limitations of the current algorithm are discussed, along with potential directions for future improvements and research avenues in DOT reconstruction methods.

2. Related Work

The reconstruction challenge of DOT has continually been a focal research area within the biomedical optics field [1-3]. Initial reconstruction techniques primarily leveraged linearized models, such as the Born and Rytov approximations, which simplify the nonlinear problem into a linear form to ease the solving process. However, these methods are effective only under minimal changes in absorption and scattering coefficients. For media with strong scattering or significant parameter variations, the quality of reconstruction notably deteriorates. To address the limitations inherent in linearized models, researchers have commenced investigations into nonlinear reconstruction techniques. Nonlinear reconstruction approaches directly tackle both the nonlinear forward and inverse problems of DOT, often employing iterative optimization strategies. Among these, gradient-based optimization methods, such as Conjugate Gradient (CG) and quasi-Newton methods (like BFGS) [4], are most used. These methods update the reconstruction results by calculating the gradient information of the objective function, offering relatively rapid convergence rates. However, due to the ill-posed nature of the DOT problem, these methods can easily converge to suboptimal solutions and are sensitive to the selection of initial values and step sizes. To enhance the stability and accuracy of reconstructions, researchers have introduced regularization techniques. Tikhonov regularization is the most classical regularization method, which suppresses oscillations and instabilities in the reconstruction results by adding an L2-norm penalty term of the parameters to the objective function. However, Tikhonov regularization tends to produce overly smoothed reconstructed images, making it difficult to preserve tissue boundaries and details. To overcome this issue, Charbonnier and others proposed Total Variation regularization, which preserves edge information by penalizing the gradient of the reconstructed image. TV regularization has achieved tremendous success in the fields of image processing and computer vision and has subsequently been introduced to DOT reconstruction [5]. Beyond TV regularization, researchers have also explored the incorporation of other types of prior information, such as L1-norm regularization and low-rank regularization. L1-norm regularization assumes that the reconstructed image is sparse within a certain transform domain, such as the wavelet domain, and obtains a sparse solution by minimizing the L1-norm of the transformation coefficients. Daubechies and others introduced the theory of compressive sensing into DOT reconstruction, demonstrating that L1-norm regularization can significantly reduce the number of required measurements [6].

Despite extensive research on DOT reconstruction, there are still challenges and opportunities for improvement. Firstly, most existing methods adopt simplified models of light propagation, such as Diffusion Approximation (DA) and Spherical Harmonics Approximation (SPN) [7]. These models have limited accuracy at tissue boundaries and regions of low scattering. To further improve reconstruction precision, there is a need to explore more accurate light transmission models, such as the Radiative Transport Equation (RTE). Secondly, the existing methods do not fully leverage prior information, and there is limited research on combining L1-norm regularization with TV
regularization for DOT reconstruction. Addressing these issues, this paper proposes a multi-measurement DOT reconstruction method based on both L1-norm and TV regularization. Building upon existing works, this method further refines the reconstruction model and optimization algorithm, aiming to achieve higher quality and more efficient reconstruction results. The next section will deduce the mathematical principles of the algorithm in detail.

3. L1 and TV Regularized DOT Reconstruction Algorithm

3.1 Forward problem model

In DOT, the transport of light through biological tissue is described by the RTE. Compared to the DA, the RTE is a more accurate model, particularly for tissue boundaries and regions with low scattering. In the frequency domain, the RTE can be expressed as follows:

\[ \hat{s} \cdot \nabla \psi(r, \hat{s}, \omega) + (\mu_a(r) + \mu_s(r)) + i\omega/c)\psi(r, \hat{s}, \omega) = \mu_s(r) \int_{4\pi} p(\hat{s}, \hat{s}')\psi(r, \hat{s}', \omega)d\Omega' + q(r, \hat{s}, \omega) \]

In this context, \( \psi(r, \hat{s}, \omega) \) represents the radiation at position \( r \) in direction \( \hat{s} \), and at angular frequency \( \omega \). The coefficients \( \mu_a(r) \) and \( \mu_s(r) \) denote the absorption coefficient and scattering coefficient, respectively. The constant \( c \) represents the speed of light. The function \( p(\hat{s}, \hat{s}') \) is the phase function describing scattering from direction \( \hat{s} \) to \( \hat{s}' \). The term \( q(r, \hat{s}, \omega) \) represents the source term. The boundary condition is given by: \( \psi(r, \hat{n}, \omega) = 0, \hat{s} \cdot \hat{n} < 0, r \in \partial \Omega \) where \( \hat{n} \) is the outward normal vector at position \( \partial \Omega \) on the boundary. The measured data can be expressed as the integral of the outgoing radiation at the detector: \( y_i = \int_{\delta \Omega > 0} \psi(r_i, \hat{s}, \omega)(\hat{s} \cdot \hat{n})d\Omega, i = 1,2,...,N_d \) where \( r_i \) denotes the position of the i-th detector, and \( N_d \) is the total number of detectors.

3.2 Mathematical Formulation of the Inverse Problem

The inverse problem in DOT can be formulated as the estimation of the absorption coefficient distribution \( \mu_a(r) \) given the measured data \( y = [y_1, y_2, ..., y_{N_d}]^T \). By introducing L1 norm and TV regularization, the reconstruction problem can be expressed as the following minimization problem:

\[ \min_{\mu_a} \frac{1}{2} \| y - F(\mu_a) \|^2 + \alpha \| \Psi \mu_a \|_1 + \beta \mathrm{TV}(\mu_a) \] (1)

Here, \( F(\mu_a) \) is the forward operator that maps the absorption coefficient to the measured data, \( \Psi \) is wavelet sparsifying transform, \( \alpha \) and \( \beta \) are regularization parameters, and \( \mathrm{TV}(\mu_a) \) represents the total variation of \( \mu_a \), defined as:

\[ \mathrm{TV}(\mu_a) = \int_{\Omega} \sqrt{(\partial_x \mu_a)^2 + (\partial_y \mu_a)^2} \, dr \] (2)

where \( \partial_x, \partial_y \) denote the partial derivatives in the x and y directions, respectively.

3.3 Semismooth Newton Method

To solve the minimization problem, we employ the semismooth Newton method. First, we introduce two auxiliary variables \( w \in R^N \) and \( v = (v_x, v_y) \in R^{2N} \), where \( N \) is the dimension of the unknown \( \mu_a \). The original problem is then transformed into:

\[ \min_{\mu_a, w, v} \frac{1}{2} \| y - F(\mu_a) \|^2 + \alpha \sum_{i=1}^{N}\left( \|w_i\| + \frac{(\Psi \mu_a)_i^2}{2 \|w_i\|} \right) + \beta \sum_{i=1}^{N}\left( \sqrt{(v_x)_i^2 + (v_y)_i^2} + \frac{(\partial_x \mu_a)_i^2 + (\partial_y \mu_a)_i^2}{2 \sqrt{(v_x)_i^2 + (v_y)_i^2}} \right) \]

We then alternately optimize \( \mu_a, w, \) and \( v \):

1. Fix \( w \) and \( v \), and update \( \mu_a \) using the Newton method:
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a. Compute the gradient:
\[
\nabla \mu_a = \int_0^1 (F(\mu_a) - y) + \alpha \Psi^T (\Psi \mu_a ./ |w|) + \beta \nabla \cdot \left( \nabla \mu_a ./ \sqrt{v_x^2 + v_y^2} \right)
\] (3)

where \( F \) is the Jacobian matrix of \( F \), and \( \nabla = (\partial_x, \partial_y)^T \).

b. Compute the approximate Hessian matrix:
\[
H_{\mu_a} \approx \int_0^1 \nabla \mu_a \Psi^T \text{diag}(1./|w|) \Psi \nabla \mu_a + \beta \nabla \cdot \text{diag}(1./\sqrt{v_x^2 + v_y^2}) \nabla \mu_a
\]

c. Update \( \mu_a \) using the Newton method:
\[
\mu_a \leftarrow \mu_a - H_{\mu_a}^{-1} \nabla \mu_a
\]

2. Update \( w \) and \( v \) based on the updated \( \mu_a \):
\[
w_i \leftarrow \frac{|\Psi \mu_a|}{\sqrt{1 + 2\alpha}}, \quad (v_x)_i \leftarrow \frac{|(\partial_x \mu_a)|}{\sqrt{1 + 2\beta}}, \quad (v_y)_i \leftarrow \frac{|(\partial_y \mu_a)|}{\sqrt{1 + 2\beta}}, \quad i = 1, 2, ..., N
\]

3. Repeat steps 1 and 2 until convergence.

Fig. 1 Mesh grid and true scattering coefficient distribution

4. Reconstruction Results and Discussion

To evaluate the performance of the algorithm proposed in this article, we designed a series of simulation experiments to verify the effectiveness and superiority of the algorithm through numerical simulations. All experiments were conducted on a computer equipped with an Intel I7-13700 processor and 64 GB of memory, running Windows 11 operating system.

We first generated synthetic data using numerical simulations. We considered a circular absorber with a diameter of 10 mm, which contains a square absorptive anomaly region measuring 1.5 mm \( \times \) 1.5 mm. The background absorption coefficient was set to 0.1 mm\(^{-1}\), and the scattering coefficient
was set to 5 mm\(^{-1}\), while the square region had an absorption coefficient of 0.2 mm\(^{-1}\), with the same scattering coefficient as the background. We uniformly placed 12 sources and 12 detectors around the surface of the circular absorber and used the RTE forward problem solver to generate measurement data. Fig. 1 gives the model used for our simulations and true scattering coefficient distribution. To simulate the noise typically present in actual measurements, we added Gaussian noise to the synthetic data.

We compared the proposed algorithm with two other methods: 1) the traditional Tikhonov regularization method; 2) L1 norm regularization method. For our algorithm, we selected the optimal regularization parameters through a grid search. The methods were tested at noise levels of 0%, 0.01%, and 0.03% to evaluate their robustness and efficacy in noise handling.

To quantitatively assess the reconstruction quality, we calculated the Relative Error (RE) and the Structural Similarity Index (SSIM) between the reconstructed and true absorption coefficients. Here, \( \mu_a \) and \( \mu_a^- \) represent the reconstructed and true absorption coefficients, respectively. \( \mu_a \) and \( \mu_a^- \) are their respective means, \( \sigma_{\mu_a} \) and \( \sigma_{\mu_a^-} \) are their standard deviations, and \( \sigma_{\mu_a \mu_a^-} \) is the covariance between them. Constants \( C_1 \) and \( C_2 \) are used to prevent division by zero in the computation. Here, \( C_1 \) is set to 1e-4 and \( C_2 \) is set to 3e-4.

\[
RE = \frac{\| \mu_a - \mu_a^- \|_2}{\| \mu_a^- \|_2} \times 100\%
\]

\[
SSIM = \frac{(2\mu_a\mu_a^- + \sigma_{\mu_a \mu_a^-})(2\sigma_{\mu_a \mu_a^-} + C_2)}{\mu_a + \mu_a^- + C_1(\sigma_{\mu_a}^2 + \sigma_{\mu_a^-}^2 + C_2)}
\]

The reconstruction results by proposed algorithm, L2 regularization and L1 regularization are shown in Fig. 2. At noise Level 0%, the reconstruction of proposed algorithm exhibits a clear delineation of the target area against the background, with virtually no artifacts and sharp edges (Fig. 1A). The result of L2 regularization is relatively smooth with slight blurring at the boundaries and details, indicating potential over-smoothing (Fig. 1B). The reconstructions L1 regularization is sparser, with fewer noise artifacts, although the reconstructed target area is smaller than actual (Fig. 1C). At noise Level 0.01%, despite the introduction of slight noise, the target area in the reconstruction of the proposed algorithm remains distinctly visible with maintained edge sharpness and contrast (Fig. 1D). Increased noise leads to further blurring of the target details and reduced contrast in L2 regularization reconstruction (Fig. 1E). Compared to L2 regularization, L1 regularization shows a slight improvement in noise handling, yet the contrast and sharpness are not as good as those achieved with our method (Fig. 1F). At noise Level 0.03%, the noise is more pronounced in the reconstructions of proposed algorithm, but the target contours remain clear, and detail is relatively well preserved (Fig. 1G). The detail and edge clarity of L2 regularization result significantly degrade, substantially affecting image quality (Fig. 1H). L1 regularization performs poorly under high noise conditions, failing to reconstruct the target area effectively (Fig. 1I).
Fig. 2 Reconstruction results by L1+TV (Column 1), L2(Column 2) and L1(Column 3) with 0%, 0.01% and 0.03% Gaussian noise respectively.

Tab. 1 shows the performance of three methods at a 0.01% noise level. Our method converges quickly, offering high-quality reconstructions and superior RE and SSIM, highlighting its efficiency and quality. L2 regularization, needing more iterations, results in higher errors and lower SSIM, with less clarity and longer computation times. L1 regularization, despite the fastest convergence, achieves the lowest quality and SSIM, failing to maintain image details effectively.

Table 1. Performance evaluation results at noise level of 0.01%

<table>
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<th>Iteration times</th>
<th>RE</th>
<th>SSIM</th>
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<td>22</td>
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<td>0.9309</td>
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<tr>
<td>L2 regularization</td>
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<tr>
<td>L1 regularization</td>
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5. Summary

This paper introduces a diffuse optical tomography reconstruction algorithm based on the semi-smooth Newton method, incorporating L1 norm and total variation regularization. Compared to existing methodologies, this algorithm demonstrates significant advantages in noise suppression, boundary preservation, and overall reconstruction quality. Nevertheless, there are certain limitations and areas for improvement. Although the L1 norm and TV regularization effectively introduce a sparse prior, they can sometimes lead to a piecewise constant effect, inadvertently smoothing over some detailed features. Future developments could also leverage parallel computing and GPU acceleration technologies to further enhance the computational efficiency and scalability of the algorithm.

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References