BSuE39.pdf

A PDE-Constrained Optimization Approach to Optical Tomography

Xuejun Gu [1,*] **and Andreas H. Hielscher** [1,2]

[1] *Department of Biomedical Engineering, Columbia University, New York, NY 10027;*
[2] *Department of Radiology, Columbia University, New York, NY 10027*
[*]xg2108@columbia.edu

Abstract: We report on the first formulation of the inverse problem in optical tomography within the framework of PDE-constrained optimization and combine Newton's method for numerical optimization with a Krylov subspace solver. This approach leads to reduced memory requirements and increased convergence speed.

OCIS codes: (000.4430) Numerical approximation and analysis (170.6960) Tomography.

1. Introduction

Still one of the major challenges in optical tomography (OT) is the development of efficient numerical algorithms for solving both the forward and inverse light propagation problems. Most algorithms currently employed in OT formulate the inverse problem as an unconstrained optimization problem [1]. In this paper, we introduce a Lagrangian approach for solving the inverse problems in optical tomography (OT), which combines the forward and inverse model under one optimization function. As a forward model of light propagation we use the radiative transport equation (RTE). The inverse problem is formulated as a minimization problem with the RTE being considered as an equality constraint on the set of "optical properties – radiance" pairs. This approach allows the incorporation of the recently developed technique of PDE-constrained optimization, which has shown great promise in many applications that can be formulated as infinite-dimensional optimization problems [2] and increase the convergence rate. Further implementing a Krylov subspace solver for the forward and inverse problem further reduces the memory requirements.

In this paper we first present the Lagrangian, KKT condition and KKT system. Subsequently the Krylov subspace solver is introduced. Using synthetic data, we present reconstructed results using the full Newton method and two of its approximations, the Gauss-Newton and the Quasi-Newton method.

2. OT On PDE Constrained Optimization Formulation

2.1. Lagrangian with Least Square Objective Function

The objective function to be minimized in optical tomography can be formulated as a least square function with N_s sources and N_d detector per source:

$$\mathscr{F}(\mu) = \frac{1}{2}\sum_{s=1}^{N_s}\sum_{d=1}^{N_s^d}\int_{\Omega}|P_d u_s - z_s^d|^2\delta(x-x_s^d)d\mathbf{x} + \beta\mathscr{R}(\mu). \tag{1}$$

where μ is the reconstructed parameter (being μ_a only, μ_s only, or both μ_a and μ_s). z_s^d is the recorded measurement on the source s, u_s is predicted radiance field. $R(\mu)$ is the regularization term and β is a regularization parameter. Details of these parameters can be found in paper [1].

The reconstruction problem can be formulated as a nonlinear constrained optimization problem writing

$$min\mathscr{F}(\mu,u); \text{ with } \; s.t.u(\mu)=0, \tag{2}$$

here $u(\mu)$ is an frequency-domain RTE defined as a complex function with a complex variable u,

$$\begin{aligned} \frac{\omega}{v}u(\mathbf{x},\theta) + (\theta\cdot\nabla + \mu_t(\mathbf{x}))u(\mathbf{x},\theta) - \mu_s(\mathbf{x})\int_{s^2}k(\theta\cdot\theta')u(\mathbf{x},\theta')\,d\theta' &= 0 \qquad \text{in } \mathscr{D}\times S^2 \\ u(\mathbf{x},\theta) &= q(\mathbf{x},\theta) \qquad \text{on } \Gamma_-; \end{aligned} \tag{3}$$

It is more convenient to separate the complex variable into real (u^R) and imaginary (u^I) parts. The Lagrangian function $\mathscr{L}(\mu,u^R,u^I,\lambda^R,\lambda^I)$ can be written as:

$$\mathscr{L}(\mu,u^R,u^I,\lambda^R,\lambda^I) = \mathscr{F}(\mu,u) + L_1(\lambda^R) + L_2(\lambda^I). \tag{4}$$

The term $\mathscr{L}_1$ and $\mathscr{L}_2$ are the integrals of the PDE over the domain:

$$L_1(\lambda^R) = \sum_{i=1}^{N_s} \left\{ \int_\Omega \int_{s^2} \lambda^R [-\frac{\omega}{v} u^I + (\theta \cdot \nabla + \mu_t(\mathbf{x})) u^R(\mathbf{x}, \theta) - \mu_s(\mathbf{x}) \int_{s^2} k(\theta \cdot \theta') u^R(\mathbf{x}, \theta')\, d\theta'] d\mathbf{x} d\theta, + \int_{\Gamma_-} \lambda^R [u^R(\mathbf{x}, \theta) - q^R(\mathbf{x}, \theta)] d\Gamma_- \right\};$$

$$L_2(\lambda^I) = \sum_{i=1}^{N_s} \left\{ \int_\Omega \int_{s^2} \lambda^I [\frac{\omega}{v} u^R + (\theta \cdot \nabla + \mu_t(\mathbf{x})) u^I(\mathbf{x}, \theta) - \mu_s(\mathbf{x}) \int_{s^2} k(\theta \cdot \theta') u^I(\mathbf{x}, \theta')\, d\theta'] d\mathbf{x} d\theta, + \int_{\Gamma_-} \lambda^I [u^I(\mathbf{x}, \theta) - q^I(\mathbf{x}, \theta)] d\Gamma_- \right\}.$$

2.2. The First Order Optimality Necessary Condition (KKT Condition) and KKT sytem

The solution to the constrained optimization problem (2) satisfied the first optimality conditions. Treating the scattering coefficient in the media as a constant and only considering to recover the absorption map, the KKT condition can be expressed as:

$$\begin{aligned} \mathscr{L}_{u^R}(u^R, u^I, \mu, \lambda^R, \lambda^I) = 0;\ & \mathscr{L}_{u^I}(u^R, u^I, \mu, \lambda^R, \lambda^I) = 0; \\ & \mathscr{L}_{\mu_a}(u^R, u^I, \mu, \lambda^R, \lambda^I) = 0; \\ \mathscr{L}_{\lambda^R}(u^R, u^I, \mu, \lambda^R, \lambda^I) = 0;\ & \mathscr{L}_{\lambda^I}(u^R, u^I, \mu, \lambda^R, \lambda^I) = 0. \end{aligned} \tag{5}$$

here $\mathscr{L}_{u^R}$ is the derivative of the lagrangian with respect to u^R, similar to u^I, μ^a, λ^R, and λ^I. The first two KKT conditions are the adjoint transport equation which project back the mismatch of the objective function to the whole computation domain. The third optimality condition here is the gradient of the Lagrangian function respective to reconstruction parameter.The forth and fifth KKT conditions are simple the forward problem of RTE.

The second derivative of Lagrangian function forms a KKT System. Here with the function expressed in Eq (4), the KKT system is:

$$\begin{bmatrix} \mathscr{L}_{u^R u^R} & 0 & \mathscr{L}_{u^R \mu_a} & \mathscr{L}_{u^R \lambda^R} & \mathscr{L}_{u^R \lambda^I} \\ 0 & \mathscr{L} u^I u^I & \mathscr{L}_{u^I \mu_a} & \mathscr{L}_{u^I \lambda^R} & \mathscr{L}_{u^I \lambda^I} \\ \mathscr{L}_{\mu_a u^R} & \mathscr{L}_{\mu_a u^R} & \mathscr{L}_{\mu_a \mu_a} & \mathscr{L}_{\mu_a \lambda^R} & \mathscr{L}_{\mu_a \lambda^I} \\ \mathscr{L}_{\lambda^R u^R} & \mathscr{L}_{\lambda^R u^I} & \mathscr{L}_{\lambda^R \mu_a} & 0 & 0 \\ \mathscr{L}_{\lambda^I u^R} & \mathscr{L}_{\lambda^I u^I} & \mathscr{L}_{\lambda^I \mu_a} & 0 & 0 \end{bmatrix} \begin{pmatrix} \bar{u}^R \\ \bar{u}^I \\ \bar{\mu}_a \\ \bar{\lambda}^R \\ \bar{\lambda}^I \end{pmatrix} = - \begin{pmatrix} \mathscr{L}_{u^R} \\ \mathscr{L}_{u^I} \\ \mathscr{L}_{\mu_a} \\ \mathscr{L}_{\lambda^R} \\ \mathscr{L}_{\lambda^I} \end{pmatrix}. \tag{6}$$

3. Optimization Schemes with a Reduced Space Method and a Krylov-Subspace Solver

The reduce space method accurately eliminates and releases some constrains and projects the updating space into the optical properties only. Cooperating the KKT conditions, in the reduced-space, KKT system becomes:

$$\begin{bmatrix} \mathscr{L}_{u^R u^R} & 0 & \mathscr{L}_{u^R \mu_a} & \mathscr{L}_{u^R \lambda^R} & \mathscr{L}_{u^R \lambda^I} \\ 0 & \mathscr{L}_{u^I u^I} & \mathscr{L}_{u^I \mu_a} & \mathscr{L}_{u^I \lambda^R} & \mathscr{L}_{u^I \lambda^I} \\ \mathscr{L}_{\mu_a u^R} & \mathscr{L}_{\mu_a u^R} & \mathscr{L}_{\mu_a \mu_a} & \mathscr{L}_{\mu_a \lambda^R} & \mathscr{L}_{\mu_a \lambda^I} \\ \mathscr{L}_{\lambda^R u^R} & \mathscr{L}_{\lambda^R u^I} & \mathscr{L}_{\lambda^R \mu_a} & 0 & 0 \\ \mathscr{L}_{\lambda^I u^R} & \mathscr{L}_{\lambda^I u^I} & \mathscr{L}_{\lambda^I \mu_a} & 0 & 0 \end{bmatrix} \begin{pmatrix} \bar{u}^R \\ \bar{u}^I \\ \bar{\mu}_a \\ \bar{\lambda}^R \\ \bar{\lambda}^I \end{pmatrix} = - \begin{pmatrix} 0 \\ 0 \\ \mathscr{L}_{\mu_a} \\ 0 \\ 0 \end{pmatrix} \tag{7}$$

Focusing on reconstructing absorption only the Newton-type updating can be written as:

$$\mu_a(k+1) = \mu_a(k) + \alpha \bar{\mu}_a. \tag{8}$$

here, α is line search step length, applied soft-line search scheme; $\bar{\mu}_a$ is the updating direction of the optical property. We have implemented three different methods for determining $\bar{\mu}_a$: Newton method, Guass-Newton method and Quasi-Newton method.

Performing the Gauss elimination of $\bar{u}$ and $\bar{\lambda}^R$ on equation (7), updating direction can be found by:

$$\mathscr{H}_{red} \bar{\mu}_a = -\mathscr{L}_{\mu_a}. \tag{9}$$

With $J = \mathscr{L}_{\lambda u}^{-1} \mathscr{L}_{\lambda \mu_a}$, the reduced Hessian $\mathscr{H}_{red}$ can be written as:

$$\mathscr{H}_{red} = \mathscr{L}_{\mu_a \mu_a} + J^T \mathscr{L}_{uu} J - J^T \mathscr{L}_{u \mu_a} - \mathscr{L}_{\mu_a u} J, \tag{10}$$

Modified the above reduced Hessian $\mathscr{H}_{red}$ to make the $\mathscr{H}_{red}$ positive definiteness, we can write the a Gauss-Newton approximation formula:

$$\mathscr{H}_{red}^{GN} = \mathscr{L}_{\mu_a\mu_a} + J^T \mathscr{L}_{uu} J. \tag{11}$$

The Quasi-Newton approximation replaces the reduced Hessian $\mathscr{H}_{red}$ with the BFGS approximation $\mathbf{B}$. Insteading of inverting the Hessian matrix, the BFGS algorithm updates the inverse Hessian $\mathbf{D} = \mathbf{B}^{-1}$ at each step. Thus search direction becomes:

$$\bar{\mu}_a(k) = -\mathscr{D}\mathscr{L}_{\mu_a(k)}. \tag{12}$$

The Krylov-subspace method finds one, or a few, eigenvalues of large sparse matrices. It is used for solving large systems of linear equations, in which it is desirable to avoid matrix-matrix operations. For finding the above inverse searching direction, a Hessian-matrix-free method is adopted. For example, in the Newton method

$$\mathscr{H}_{red}\bar{\mu}_a = \mathscr{L}_{\mu_a\mu_a}\bar{\mu}_a + J^T \mathscr{L}_{uu} J\bar{\mu}_a - J^T \mathscr{L}_{u\mu_a\bar{\mu}_a} - \mathscr{L}_{\mu_a u} J\bar{\mu}_a. \tag{13}$$

Introduce two auxiliary variables Y_1 and Y_2, the above equation (13) can be split into the following three equations, which can be solved iteratively: $\mathscr{L}_{\lambda u}Y_1 = \mathscr{L}_{\lambda\mu_a}\bar{\mu}_a$; $\mathscr{L}_{u\lambda}Y_2 = \mathscr{L}_{uu}Y_1 - \mathscr{L}_{u\mu_a}\bar{\mu}_a$; and $\mathscr{H}_{red}\bar{\mu}_a = \mathscr{L}_{\mu_a\mu_a}\bar{\mu}_a + \sum_{s=1}^{N_s}\mathscr{L}_{\mu_a\lambda}Y_2 - \mathscr{L}_{\mu_a u}Y_1$;

4. Numerical Results

We have extensively tested the three different reduced-space methods within the framework PDE-constrained optimization. An example is shown in Figure 1, where we simulated measurements on a $2cm \times 2cm$ domain descritized as 81×81 grids that contains a target with an absorption coefficient twice as high as the coefficient for the background. The scattering coefficient is $50.0cm^{-1}$ and g=0.9. For the reconstruction we used data from 4 sources and 156 detectors, equally spaced around the phantom. (see the exact setup in Fig 1– Exact Setup). For this example the source modulation frequency was 500 MHz. Fig. 1 displays the 2D reconstructed results as well as the μ_a-values along lines that cross the center of the inhomogeneity along the x and y-axis.

Overall we found that using the PDE-constrained approach together with the Krylov-subspace method, the computational memory can be saved with a factor of the square root of the memory used in non-Krylov method. Depending on the particular problem considered, we observed speed increase between a factor of 5 and 20. Also, using the framework of the Lagrangian function, all other boundary constrained conditions can be added without further remodelling.

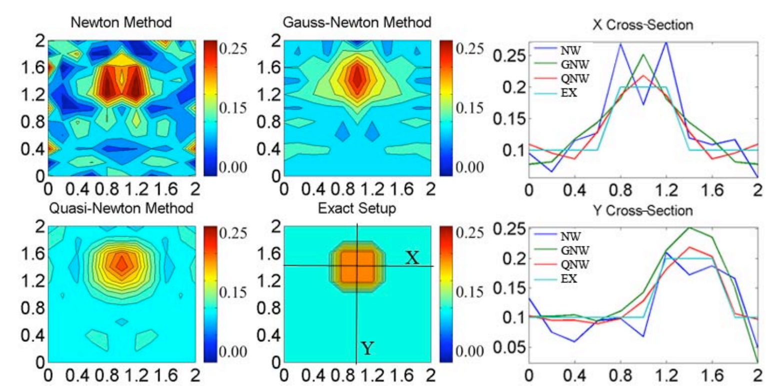

Figure 1. An example of the reconstruction results with variants Newton-type methods

This work was supported in part by the National Institute of Arthritis and Musculoskeletal and Skin Diseases (NIAMS-2R01-AR046255) and the National Institute of Biomedical Imaging and Bioengineering (NIBIB-R01EB001900), which are both divisions of the National Institutes of Health (NIH).

References

[1] K. Ren, G. S. Abdoulaev, G. Bal, and A. H. Hielscher. "'requency-domain optical tomography with the equation of radiative transfer."' *SIAM Journal on Scientific Computing(SISC)*, 28(4):1463–1489, 2006.

[2] G. Abdoulaev, K. Ren, and A. H. Hielscher. "'Optical tomography as a constrained optimization problem."' *Inverse Problem*, 21:1507–1530, 2005.