QPATDiff.m: Quantitative Photoacoustic Tomography Based on the Diffusion Model

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Overview. This is a MATLAB code for solving the inverse problem in quantitative photoacoustic tomography based on the diffusion model for light propagation.

Mathematical Model. The mathematical model is the following boundary value problem for the diffusion equation

$$-\nabla\cdot\gamma\nabla u+\sigma u=0,\quad \text{in}\ \ \Omega,\qquad \boldsymbol{\nu}\cdot\gamma\nabla u(\mathbf{x})+\kappa u=f(\mathbf{x}),\quad \text{on}\ \ \partial\Omega \tag{1}$$

The Robin boundary condition here makes this diffusion model more realistic than the Dirichlet boundary condition used in [1]. It also prevents us from using the vector-field based reconstruction method in [1]. Instead, we use a minimization based method here like the one in [4].

It is important to notice that the diffusion coefficient γ appears in both the equation and the boundary condition. This induces a boundary term in the Fréchet derivative of the objective function for γ which cancels out another boundary term coming out of integration by part. This makes the derivative with respect to γ very simple.

The Data. The data we measure are encoded in the map:

$$\Lambda_{\Gamma,\gamma,\sigma}: f(\mathbf{x})\mapsto H(\mathbf{x}):=\Gamma\sigma u \tag{2}$$

The Domain. The computational domain is $\Omega=(0,2)\times(0,2)$.

The Objective. The objective here is to reconstruct some information on (Γ,γ,σ) from data encoded in $\Lambda_{\Gamma,\gamma,\sigma}$. According to the theory of [1, 2] unless multi-spectral data are available. We therefore can only hope to reconstruct at most two of the three coefficients.

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The Algorithm. We assume that we collect data from N_s illuminations $\{f_j\}_{j=1}^{N_s}$. The diffusion equation for source f_j is

$$-\nabla\cdot\gamma\nabla u_j+\sigma u_j=0,\quad\text{in}\quad\Omega,\qquad \boldsymbol{\nu}\cdot\gamma\nabla u_j(\mathbf{x})+\kappa u_j=f_j(\mathbf{x}),\quad\text{on}\quad\partial\Omega \tag{3}$$

The corresponding data is $H_j(\mathbf{x})=\Lambda_\sigma f_j:=\Gamma\sigma u_j$. We therefore collected data $\{f_j,H_j(\mathbf{x})\}_{j=1}^{N_s}$.

We solve the inverse problem is in least-square form. We minimize

$$\Phi(\Gamma,\gamma,\sigma):=\frac{1}{2}\sum_{j=1}^{N_s}\int_\Omega(\Gamma\sigma u_j-H_j)^2d\mathbf{x}+\frac{\beta}{2}\int_\Omega\left[|\nabla\Gamma|^2+|\nabla\gamma|^2+|\nabla\sigma|^2\right]d\mathbf{x} \tag{4}$$

where the parameter β is the strength of the regularization term. Note that, the regularization functional should only contain terms for quantities to be reconstructed. For instance, if we only reconstruct σ, then $|\nabla\sigma|^2$ should be the only term in the regularization functional.

The Gradient Calculation. We use the adjoint state method to calculate the gradient of the objective functional with respect to the absorption coefficient σ. Let w_j $(1\le j\le N_s)$ be the solution to adjoint equation

$$-\nabla\cdot\gamma\nabla w_j+\sigma w_j=-(\Gamma\sigma u_j-H_j)\Gamma\sigma,\quad\text{in}\quad\Omega,\qquad \boldsymbol{\nu}\cdot\gamma\nabla\ w_j+\kappa w_j=0,\quad\text{on}\quad\partial\Omega \tag{5}$$

We can then show that the Fréchet derivatives of Φ are given as

$$\begin{aligned}\Phi'(\Gamma,\gamma,\sigma)[\delta\Gamma]=&\sum_{j=1}^{N_s}\int_\Omega(\Gamma\sigma u_j-H_j)\sigma u_j\delta\Gamma(\mathbf{x})d\mathbf{x}\\&-\beta\Big[\int_\Omega(\Delta\Gamma)\delta\Gamma(\mathbf{x})d\mathbf{x}-\int_{\partial\Omega}\partial_\nu\Gamma\delta\Gamma(\mathbf{x})dS(\mathbf{x})\Big].\end{aligned} \tag{6}$$

$$\begin{aligned}\Phi'(\Gamma,\gamma,\sigma)[\delta\gamma]=&\sum_{j=1}^{N_s}\int_\Omega\nabla u_j\cdot\nabla w_j\delta\gamma d\mathbf{x}\\&-\beta\Big[\int_\Omega(\Delta\gamma)\delta\gamma(\mathbf{x})d\mathbf{x}-\int_{\partial\Omega}\partial_\nu\gamma\delta\gamma(\mathbf{x})dS(\mathbf{x})\Big].\end{aligned} \tag{7}$$

$$\begin{aligned}\Phi'(\Gamma,\gamma,\sigma)[\delta\sigma]=&\sum_{j=1}^{N_s}\int_\Omega\left[(\Gamma\sigma u_j-H_j)\Gamma u_j+u_jw_j\right]\delta\sigma d\mathbf{x}\\&-\beta\Big[\int_\Omega(\Delta\sigma)\delta\sigma(\mathbf{x})d\mathbf{x}-\int_{\partial\Omega}\partial_\nu\sigma\delta\sigma(\mathbf{x})dS(\mathbf{x})\Big].\end{aligned} \tag{8}$$

The boundary integral terms will disappear if we assume that the boundary values of the coefficients are known.

The Forward/Adjoint Solver. In the minimization process, we solve the forward and adjoint diffusion problems (3) and (5) with a standard P_1 finite element solver of the MATLAB PDE Toolbox.

This code was a simplification of the code we used to generate some of the numerical results in [4] and [3]. We replaced the optimization algorithms with a MATLAB `fminunc` algorithm.

Remark on the objective function. Optical signals decay fast away from the source location. It is thus very useful to normalize the data whenever possbile. For instance, the following normalized objective function works very well when $H_j > 0$ everywhere:

$$\Phi(\Gamma, \gamma, \sigma) := \frac{1}{2} \sum_{j=1}^{N_s} \int_\Omega (\Gamma \sigma u_j - H_j)^2 d\mathbf{x} + \text{regularization} \tag{9}$$

The adjoint problem as well as the derivatives for this normalized objective function can be written down similarly. The code have both the normalized and the unnormalized objective functions.

References

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