# On multi-spectral quantitative photoacoustic tomography

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The objective of quantitative photoacoustic tomography (qPAT) is to reconstruct the diffusion, absorption and thermal expansion coefficients of heterogeneous media from knowledge of the interior absorbed radiation. It has been shown [1] that with data acquired at one given wavelength, all three coefficients cannot be reconstructed uniquely. In this Letter, we study the multi-spectral qPAT problem and show that when multiple wavelength data are available, all coefficients can be reconstructed simultaneously under minor prior assumptions. Moreover, the reconstructions are shown to be very stable. We present numerical simulations that support the theoretical results. 

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In photoacoustic tomography, near infra-red (NIR) light propagates into a medium of interest. As a fraction of the incoming light energy is absorbed, the medium heats up. This results in mechanical expansion and the generation of compressive (acoustic) waves. The acoustic waves propagate to the boundary of the medium where they are measured. From the knowledge of these (time-dependent) acoustic measurements, qPAT attempts to reconstruct the absorption, scattering and thermal expansion properties of the medium of interest [2,3].

The reconstruction problem in photoacoustic tomography is a two-step process. In the first step, one reconstructs the absorbed energy map $H(\mathbf{x})$ defined in (2) below from the measured acoustic signals on the surface of the medium. This is a relatively well known inverse source problem for the wave equation that has been extensively studied in the past [4,5]. In the second step, the objective is to reconstruct the diffusion, absorption and Grüneisen thermal expansion coefficients from the reconstructed energy data $H(\mathbf{x})$. This step has been studied only more recently [1,6,7].

Let us denote by $X$ a bounded domain in $\mathbb{R}^d$ $(d = 2, 3)$ with smooth boundary $\partial X$, and $\Lambda \subset \mathbb{R}_+$ the set of wavelengths at which the interior data are constructed. In the diffusive regime, the density of photons at wavelength $\lambda$, $u(\mathbf{x}, \lambda)$ solves the following diffusion equation

$$\begin{aligned} -\nabla \cdot D(\mathbf{x},\lambda)\nabla u(\mathbf{x},\lambda) + \sigma(\mathbf{x},\lambda)u = 0, &\quad X \times \Lambda \\ u(\mathbf{x},\lambda) = g(\mathbf{x},\lambda), &\quad \partial X \times \Lambda \end{aligned} \tag{1}$$

where $D(\mathbf{x}, \lambda) > 0$ and $\sigma(\mathbf{x}, \lambda) > 0$ are the wavelength-dependent diffusion and absorption coefficients, respectively, and $g(\mathbf{x}, \lambda)$ is the illumination pattern in photoacoustic experiments. The wavelength-dependent interior data constructed from the inversion of the acoustic problem are given by

$$H(\mathbf{x},\lambda) = \Gamma(\mathbf{x},\lambda)\sigma(\mathbf{x},\lambda)u(\mathbf{x},\lambda), \quad (\mathbf{x},\lambda) \in X \times \Lambda \tag{2}$$

where $\Gamma(\mathbf{x}, \lambda) > 0$ is the Grüneisen coefficient that measures the (non-dimensionalized) thermal expansion rate of the medium when it heats up.

The problem of qPAT is to reconstruct the coefficients $D(\mathbf{x}, \lambda)$, $\sigma(\mathbf{x}, \lambda)$ and $\Gamma(\mathbf{x}, \lambda)$ from interior data of the form (2). The results in [1] state that without further *a priori* information, we cannot uniquely reconstruct all three coefficients. In fact, only two quantities related to the three coefficients, i.e., the functionals $\mu(\mathbf{x}, \lambda)$ and $q(\mathbf{x}, \lambda)$ defined in (5) below can be reconstructed. The objective of this Letter is to show that when data of multiple wavelengths are available, we can recover the uniqueness in the reconstructions with relatively little additional *a priori* information. We allow the diffusion and absorption coefficients to be arbitrary functions of the wavelength and assume that the Grüneisen coefficient can be written as the product of a function of space and a function of wavelength. More precisely, the coefficients take the following form:

$$D = D(\mathbf{x},\lambda), \quad \sigma = \sigma(\mathbf{x},\lambda), \quad \Gamma(\mathbf{x},\lambda) = \gamma(\lambda)\Gamma(\mathbf{x}) \tag{3}$$

where $\gamma(\lambda)$ is a function assumed to be *known*. This assumption is not sufficient to guaranty unique reconstructions. We need to assume a little more on the coefficients. Our main assumption is:

(**A1**). There exist two *known* wavelengths $\lambda_1, \lambda_2 \in \Lambda$ so that $D(\mathbf{x}, \lambda_1) = \rho D(\mathbf{x}, \lambda_2)$ for some *known* positive constant $\rho$, while $\frac{\sigma}{\sqrt{D}}(\mathbf{x}, \lambda_1) \neq \frac{\sigma}{\sqrt{D}}(\mathbf{x}, \lambda_2)$ for all $\mathbf{x} \in X$.

This assumption essentially requires that the dependence of the diffusion and absorption coefficients is different for at least two wavelengths. We also need some assumptions on the regularity and boundary values of the coefficients. We assume, denoting by $\mathcal{C}^p(X)$ the space of $p$-times differentiable functions in $X$, that

(**A2**). The function $0 < D(\cdot, \lambda) \in \mathcal{C}^2(\bar{X})$, and its boundary value $D|_{\partial X}$ is *known*. The functions $0 < \sigma(\cdot, \lambda), 0 < \Gamma(\cdot, \lambda) \in \mathcal{C}^1(\bar{X})$.

We now present the main uniqueness result on reconstructions with multi-spectral data.

**Theorem 1.** *Let* $(D, \sigma, \Gamma)$ *and* $(\tilde{D}, \tilde{\sigma}, \tilde{\Gamma})$ *be two sets of coefficients given in* (3), *with* $\gamma(\lambda)$ *known, satisfying the assumptions* (**A1**) *and* (**A2**). *Then there exists a open set of illuminations* $\big(g_1(\mathbf{x}, \lambda),\ g_2(\mathbf{x}, \lambda)\big)$ *such that the equatility of the data*

$$\{H_1(\mathbf{x}, \lambda),\ H_2(\mathbf{x}, \lambda)\} = \{\tilde{H}_1(\mathbf{x}, \lambda),\ \tilde{H}_2(\mathbf{x}, \lambda)\}$$

*in* $X \times \Lambda$ *implies that*

$$\{D(\mathbf{x}, \lambda),\ \sigma(\mathbf{x}, \lambda),\ \Gamma(\mathbf{x})\} = \{\tilde{D}(\mathbf{x}, \lambda),\ \tilde{\sigma}(\mathbf{x}, \lambda),\ \tilde{\Gamma}(\mathbf{x})\}$$

*in* $X \times \Lambda$ *provided that the boundary values of the diffusion coefficient agree on the boundary:* $D|_{\partial X} = \tilde{D}|_{\partial X}$ *for all* $\lambda \in \Lambda$.

*Proof.* With the regularity assumptions on the diffusion coefficient, we can recast equation (1), using the Liouville transform $v = \sqrt{D}u$, as

$$\begin{array}{rl} \Delta v(\mathbf{x}, \lambda) + q(\mathbf{x}, \lambda) v(\mathbf{x}, \lambda) = 0, & X \times \Lambda \\ v(\mathbf{x}, \lambda) = \tilde{g}(\mathbf{x}, \lambda) := \sqrt{D}(\mathbf{x}, \lambda) g(\mathbf{x}, \lambda), & \partial X \times \Lambda \end{array} \qquad (4)$$

with the interior data $H(\mathbf{x}, \lambda) = v(\mathbf{x}, \lambda)/\mu(\mathbf{x}, \lambda)$, where $\mu$ and $q$ are defined respectively as

$$\mu = \frac{\sqrt{D}}{\Gamma\sigma}, \qquad -q = \frac{\Delta\sqrt{D}}{\sqrt{D}} + \frac{\sigma}{D}. \qquad (5)$$

Let us denote by $v_1(\mathbf{x}, \lambda)$ and $v_2(\mathbf{x}, \lambda)$ the solutions of (4) with illuminations $\tilde{g}_1(\mathbf{x}, \lambda)$ and $\tilde{g}_2(\mathbf{x}, \lambda)$ respectively. Then it is straightforward to check that

$$\begin{array}{rcl} -\nabla \cdot v_1^2 \nabla \dfrac{v_2}{v_1} & = & 0, \quad X \times \Lambda \\ v_1^2(\mathbf{x}, \lambda) & = & \tilde{g}_1^2, \quad \partial X \times \Lambda. \end{array} \qquad (6)$$

Since $\frac{v_2}{v_1} = \frac{H_2}{H_1}$ is known, this is a transport equation for $v_1^2(\mathbf{x}, \lambda)$ with the vector field $\nabla \frac{H_2}{H_1}$. By the results of [1], there exist well-chosen illuminations $g_1$ and $g_2$ such that the vector field is smooth enough with positive modulus $|\nabla \frac{H_2}{H_1}| > 0$. This ensures that the transport equation is uniquely solvable for $v_1^2$. Once $v_1^2$ is reconstructed, we can reconstruct $\mu = v_1/H_1$ and then $q = -\Delta v_1/v_1$.

Now let $\lambda_1,\ \lambda_2 \in \Lambda$ be two wavelengths as in assumption (**A1**). We first reconstruct the two pairs of functionals $(\mu(\mathbf{x}, \lambda_1),\ q(\mathbf{x}, \lambda_1))$ and $(\mu(\mathbf{x}, \lambda_2),\ q(\mathbf{x}, \lambda_2))$. With the assumption that $D(\mathbf{x}, \lambda_1) = \rho D(\mathbf{x}, \lambda_2)$, we obtain after some algebra using the above equations that

$$\begin{array}{rl} \Delta\sqrt{D}(\mathbf{x}, \lambda_1) + Q(\mathbf{x})\sqrt{D}(\mathbf{x}, \lambda_1) = 0, & X \\ \sqrt{D}(\mathbf{x}, \lambda_1) = \sqrt{D}(\mathbf{x}, \lambda_1)_{|\partial X}, & \partial X \end{array} \qquad (7)$$

where the function $Q(\mathbf{x})$ is defined as $Q(\mathbf{x}) = \dfrac{\gamma(\lambda_1)\mu(\mathbf{x}, \lambda_1)q(\mathbf{x}, \lambda_1) - \sqrt{\rho}\gamma(\lambda_2)\mu(\mathbf{x}, \lambda_2)q(\mathbf{x}, \lambda_2)}{\gamma(\lambda_1)\mu(\mathbf{x}, \lambda_1) - \sqrt{\rho}\gamma(\lambda_2)\mu(\mathbf{x}, \lambda_2)}$. Using the conditions in assumptions (**A1**) and (**A2**), the denominator in $Q$ does not vanish and $Q$ is bounded. The elliptic equation (7) can then be solved uniquely as shown in [1] to reconstruct $\sqrt{D}(\mathbf{x}, \lambda_1)$. We then find

$$\sigma(\mathbf{x}, \lambda_1) = -(Dq)(\mathbf{x}, \lambda_1) - (\sqrt{D}\Delta\sqrt{D})(\mathbf{x}, \lambda_1), \qquad (8)$$

$$\Gamma(\mathbf{x}) = \frac{\sqrt{D}(\mathbf{x}, \lambda_1)}{\mu(\mathbf{x}, \lambda_1)\sigma(\mathbf{x}, \lambda_1)}. \qquad (9)$$

Once $\Gamma(\mathbf{x})$ is reconstructed, then so is $\Gamma(\mathbf{x}, \lambda) = \Gamma(\mathbf{x})\gamma(\lambda)$. The results in [1, Corollary 2.3] then allow us to reconstruct $D(\mathbf{x}, \lambda)$ and $\sigma(\mathbf{x}, \lambda)$ for all $\lambda \in \Lambda$. ☐

The proof is constructive and provides an explicit procedure to reconstruct the unknown coefficients. The main step is to solve the transport equation (6) for $v_1^2$. It has been shown in [1] that the reconstruction of $v_1$ (and thus that of $\mu$ and $q$ as well) is Lipschitz stable for each fixed wavelength. Because the solution of (7) is stable with respect to $Q$, we deduce that the reconstruction of the $D(\mathbf{x}, \lambda_1)$ (and thus $\Gamma(\mathbf{x})$) is stable. Precise stability estimates similar to those in [1, Theorem 2.4] can be derived.

The coefficient model (3) is quite general and covers many of the models used in the literature. For instance, we may consider the following standard model:

$$\begin{array}{c} D(\mathbf{x}, \lambda) = \alpha(\lambda)D(\mathbf{x}), \quad \Gamma(\mathbf{x}, \lambda) = \gamma(\lambda)\Gamma(\mathbf{x}) \\ \sigma(\mathbf{x}, \lambda) = \sum_{k=1}^{K} \beta_k(\lambda)\sigma_k(\mathbf{x}) \end{array} \qquad (10)$$

where the functions $\alpha(\lambda)$, $\{\beta_k(\lambda)\}_{k=1}^{K}$ and $\gamma(\lambda)$ are assumed to be *known*. In other words, all three coefficient functions can be written as products of functions of different variables. Moreover, the absorption coefficient contains multiple components. This is the parameter model proposed in [2,6,8–10] to reconstruct chromophore concentrations from photoacoustic measurements. The following result regarding model (10) is a natural extension of Theorem 1.

**Corollary 2.** *Let* $D(\mathbf{x}, \lambda)$, $\sigma(\mathbf{x}, \lambda)$ *and* $\Gamma(\mathbf{x}, \lambda)$ *be as in* (10) *and satisfying assumptions ((***A1***) and (***A2***). Assume further that there exist* $K$ *wavelengths such that the matrix* $B$ *with elements* $B_{kj} = \beta_k(\lambda_j)$ $(1 \le k, j \le K)$ *is non-singular. Then the coefficients*

$$\{D(\mathbf{x}),\ \{\sigma_k(\mathbf{x})\}_{k=1}^{K},\ \Gamma(\mathbf{x})\}$$

*can be uniquely reconstructed.*

*Proof.* Theorem 0.1 allows the unique reconstruction of $D(\mathbf{x})$, $\Gamma(\mathbf{x})$ and $\{\sigma(\mathbf{x}, \lambda_k)\}_{k=1}^{K}$. Since $B$ is non-singular, we can invert the linear system $\sigma(\mathbf{x}, \lambda_j) = \sum_{k=1}^{K} \beta_k(\lambda_j)\sigma_k(\mathbf{x})$, $j = 1, \cdots, K$ to recover $\{\sigma_k(\mathbf{x})\}_{k=1}^{K}$. ☐

The uniqueness proofs presented above are valid only for diffusion coefficients that are $\mathcal{C}^2$ in space. For problems with discontinuous diffusion coefficients, we resort to numerical algorithms that are based on optimization techniques. We look for the coefficients in the form of (3)

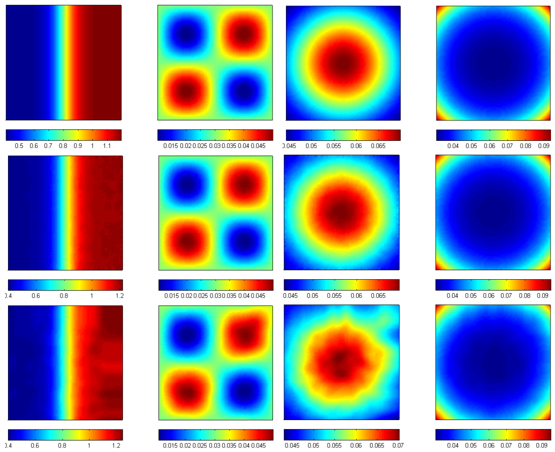

Fig. 1. Reconstruction of $(\Gamma(\mathbf{x}), D(\mathbf{x}), \sigma_1(\mathbf{x}), \sigma_2(\mathbf{x}))$. Top to bottom: true coefficients, reconstructions with clean data and those with data containing 5% random noise.

that minimize the following mismatch functional

$$\Phi(D, \sigma, \Gamma) \equiv \sum_{i=1}^{2} \|H_i(\mathbf{x}, \lambda) - H_i^*(\mathbf{x}, \lambda)\|^2_{L^2(X\times\Lambda)} \qquad (11)$$

where $H_i(\mathbf{x}, \lambda) = \Gamma(\mathbf{x}, \lambda)\sigma(\mathbf{x}, \lambda)u_i(\mathbf{x}, \lambda)$ with $u_i(\mathbf{x}, \lambda)$ the solution of the diffusion equation (1) with the $i$th source, $g_i(\mathbf{x}, \lambda)$ and $H_i^*(\mathbf{x}, \lambda)$ is the corresponding "measured" interior data. Let us denote by $w_i(\mathbf{x}, \lambda)$ be the solution of the adjoint problem

$$\begin{aligned} -\nabla \cdot D(\mathbf{x}, \lambda)\nabla w_i(\mathbf{x}, \lambda) + \sigma(\mathbf{x}, \lambda)w_i &= \Gamma\sigma Z_i, \quad X \times \Lambda \\ w_i(\mathbf{x}, \lambda) &= 0, \quad \partial X \times \Lambda \end{aligned}$$

with $Z_i \equiv H_i(\mathbf{x}, \lambda) - H_i^*(\mathbf{x}, \lambda)$. Then it is easy to show that the Fréchet derivatives of the objective functional are given by, respectively

$$\begin{aligned} &\langle \tfrac{\partial\Phi}{\partial D}, \hat{D}\rangle = \sum\langle\nabla u_i \cdot \nabla w_i, \hat{D}\rangle, \ \langle \tfrac{\partial\Phi}{\partial\Gamma}, \hat{\Gamma}\rangle = \sum\langle Z_i\sigma u_i, \hat{\Gamma}\rangle \\ &\langle \tfrac{\partial\Phi}{\partial\sigma}, \hat{\sigma}\rangle = \sum\langle \Gamma Z_i u_i - w_i u_i, \hat{\sigma}\rangle \end{aligned}$$

with $\langle\cdot\rangle$ denoting the usual inner product in $L^2(X \times \Lambda)$. High order Fréchet derivatives can be computed as well. We then use quasi-Newton algorithm implemented in [11] to minimize the functional.

We now show some two-dimensional numerical simulations in the square: $X = (0,\ 2) \times (0,\ 2)$. We attempt to reconstruct the coefficients given in (10) with two components in the absorption coefficient, i.e. $K = 2$. Other parameters are given as follows:

$$\alpha(\lambda) = \lambda^{3/2}, \quad \gamma(\lambda) = 1, \quad \beta_1(\lambda) = \lambda, \quad \beta_2(\lambda) = \lambda^{-1}.$$

Four illuminations are used, two at each wavelength. We show in Fig. 1 typical reconstructions of the four smooth coefficients $D(\mathbf{x})$, $\Gamma(\mathbf{x})$, $\sigma_1(\mathbf{x})$ and $\sigma_2(\mathbf{x})$, and in Fig. 3 typical reconstructions of piecewise smooth coefficients, the later being done with the numerical minimization algorithm mentioned above. As can be seen in

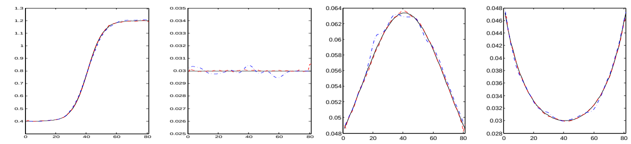

Fig. 2. Cross-sections of plots in Fig. 1 along axis $y = 1.0$. Shown are true coefficients(solid line), reconstruction with noise-free data (blue dashed) and reconstructions with noisy data (red dashed).

the cross-section plots in Fig. 2, the reconstructions are very accurate, with overall quality very similar to those presented in [1]. More systematic simulation results will be presented elsewhere. This work is supported in part

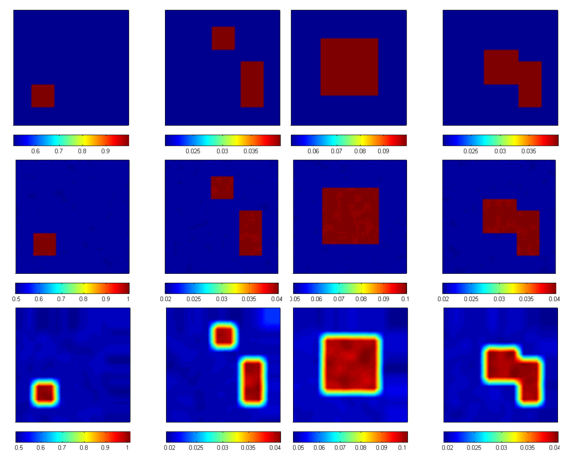

Fig. 3. Same as in Fig. 1 but for discontinuous coefficients.

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