SENSITIVITY COMPUTATIONS FOR ELLIPTIC EQUATIONS WITH INTERFACES

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Summary. In this paper we consider an inverse problem motivated by the use of electroencephalogram (EEG) data to estimate the location and strength of a neural activity in brain tissue. This problem leads to a Poisson type equation with interfaces where the source of activity is described by a model whose parameters must be estimated. Much of the work in this is based on modelling the source as a "dipole" and least square or maximum likelihood estimators are used to identify the parameters. In this paper we present a simple model to illustrate some of the theoretical and numerical issues associated with computing sensitivities for problems of this type.

1 Introduction

The problem of estimating the location and strength of a neural activity in the brain tissue from electroencephalogram (EEG) and / or magneto-electroencephalogram (MEG) measurements on the scalp has spawned considerable interest in inverse problems for multi-layered interface problems (see [5], [7], [8], [9], and [15]). One cause of an epileptic seizure is a spontaneous brain activity and accurately locating the position of this source is helpful in several proposed medical procedures to address the problem. The basic mathematical model is a Poisson equation with interfaces and leads to an elliptic equation with discontinuous coefficients due to the different conductivity values for the brain, skull and scalp. The forward problem is well understood and issues such as head shapes and movements have been carefully studied (see [9], [12], [13], [14], and [15]). Moreover, efficient numerical methods have been developed for the forward and inverse problems with interfaces and singular sources (see [6], [8], [12] and [13]). The source of often assumed to be a dipole of some type and it has been suggested that mathematical dipoles are adequate models for source generators. Nehorai and co-workers [9] have studied the inverse problem for this class of models and derived Cramer-Rao bounds which are useful in evaluating parameter estimation algorithms. Much of this theory and most numerical algorithms require the computation of sensitivities or generalized sensitivities that define the Fisher information matrix (see [9] and [11]).

In this short note we discuss the problem of constructing accurate numerical methods for sensitivity computations. We note that the problem of computing sensitivities with respect to interface locations leads to a very weak elliptic problem that requires special methods in order to achieve accurate solutions across the interfaces. Also, as noted in [6] the problem is made more difficult when the source term is singular (e.g. a delta function or dipole). We present a theoretical framework that can be used to develop approximation schemes for sensitivity computations for such equations and present numerical results to illustrate the ideas.

2 The Model

The head, denoted by G, is usually described as three homogeneous sets, one surrounded by the next one, denoted by: G_1 the brain, G_2 the skull and G_3 the scalp. The surface between them are denoted by S_1, S_2 and S_3, respectively and $S_3 = \partial G$. The conductivity function $\kappa(x)$ that contains the conductivity of the different tissues is a positive and piecewise constant function of the form

$$\kappa(x) = \sigma_j \qquad x \in G_j\,, \quad j = 1, 2, 3.$$

The Electroencephalogram (EEG) problem is modelled by a Poisson type equation of the form

$$\nabla \cdot (\kappa(x)\nabla w(x)) = F(x) \qquad x \in G \tag{1}$$

with Neumann boundary condition

$$\frac{\partial w(x)}{\partial \nu} = 0, \qquad x \in \partial G \tag{2}$$

subject to the interface conditions

$$[w]\Big|_{S_i} = 0, \qquad [\kappa(x)\frac{\partial w}{\partial \nu}]\Big|_{S_i} = 0. \tag{3}$$

The unknown $w(\cdot)$ is the electric potential, the function $\kappa(x)$ contains the conductivity values of the different tissues of the human head G, $F(x) = \nabla \cdot J_i(x)$ where $J_i(x)$ is the impressed current and ν is the external normal vector. The impressed current is supposed to be concentrated to a very small area.

The surface potential $w(\cdot)|_{G3}$ is measured as a difference between a reference point $x_0 \in \partial G$ and hence we set $w(x_0) = 0$ and this provides a boundary condition

$$w(x_0) = 0 \qquad x_0 \in \partial G. \tag{4}$$

The forward problem in EEG consists in finding the electric potential $w(\cdot)$ when $F(x)$ is given while the inverse problem consists in finding the location and strength of the source for a given potential distribution.

The source is often modelled by a dipole of current density (see [5] and [9])

$$J_i(x) = J(x, q, p) = q\delta(x - p) \tag{5}$$

and the inverse problem to to estimate the parameters q and p from scalp measurements. In addition, one also needs to have estimates of the coefficients σ_i, $i = 1, 2, 3$ and interface locations S_i, $i = 1, 2$. Moreover, the brain tissue is inhomogeneous and anisotropic and in the real problem these features require special computational methods (see [15]).

The existence of weak solutions for (1)-(4) and the continuity of the solutions with respect to the radii R_i of the sets G_i can be found in [12]. The continuity of the solutions with respect to the values of $\kappa(x)$ was stated in [13]. As noted above, the inverse problem requires the computation of sensitivities of the solution $w(\cdot)$ with respect to the "parameters" q, p, σ_i, $S_i, i = 1, 2, 3$. In this short note we limit our discussion to simplified 1D versions of the EEG Problem. The full 3D version will appear in a future paper.

3 A 1D Model Problem

Let $0 < R_1 < R_2$ and set $G = (0, R_2) = (0, R_1) \cup (R_1, R_2) = G_1 \cup G_2$ and set $\mathbf{q} = (q_1, q_2, q_3, q_4) = (\sigma_1, \sigma_2, R_1, R_2)$. We consider the elliptic interface problem

$$-\frac{\partial}{\partial x}(k(x, \mathbf{q})\frac{\partial w}{\partial x}(x, \mathbf{q})) = 0 \qquad x \in (0, q_4) \tag{6}$$

with boundary conditions

$$w(0) = 0 \tag{7}$$

and interface conditions

$$(\kappa \tfrac{\partial w}{\partial \nu})(q_3^-) = (k \tfrac{\partial w}{\partial \nu})(q_3^+), \qquad w(q_3^-) = w(q_3^+) \tag{8}$$

where $k(x, \mathbf{q})$ is the piecewise constant function

$$k(x, \mathbf{q}) = \begin{cases} q_1 & 0 < x < q_3 \\ q_2 & q_3 < x < q_4 \end{cases} . \tag{9}$$

In order to keep the paper short and to focus on the sensitivity computation, we limit our discussion to the case where the source $F(x) = 0$ and the boundary condition at R_2 is defined by

$$w(R_2) = 1. \tag{10}$$

This problem is sufficient to illustrate the nature of the sensitivity equations for various parameters such as conductivity and interface locations.

Remark. The problem with a singular source $F(x) \neq 0$ and boundary condition $w'(R_2) = 0$ is closer to the EEG problem and will be discussed in a future paper. However, it is worthwhile to note that source location identifiability is highly dependent on the choice of the model for the source $F(x)$ (see [3] and [4]). Dipole sources alone may lead to highly ill-conditioned inverse problem requiring some type of regularization.

The four parameters in the problem are the spatial location of the interface, q_3, the endpoint of the domain, q_4, that satisfies $0 < q_3 < q_4$, and the parameters $q_1 > 0, q_2 > 0$ which are the values of k on each subinterval. The solution $w(x, \mathbf{q})$ of (6)-(10) can be calculated analytically and is given by

$$w(x, \mathbf{q}) = \begin{cases} \frac{q_2}{q_2 q_3 - q_1 q_3 + q_4 q_1} & x \\ \frac{q_1}{q_2 q_3 - q_1 q_3 + q_4 q_1} & (x - q_4) + 1 \end{cases} . \tag{11}$$

Note that the denominator $q_2 q_3 - q_1 q_3 + q_4 q_1 = q_1(q_4 - q_3) + q_2 q_3$ is never zero since both terms in the right side are positive. Observe that the sensitivities $s_i(x, \mathbf{q}) = \frac{\partial w(x,\mathbf{q})}{\partial q_i}$ can also be given in explicit analytical form. For example,

$$s_1(x, \mathbf{q}) = \begin{cases} \frac{q_2(q_3 - q_4)}{(q_2 q_3 - q_1 q_3 + q_4 q_1)^2} & x & x \in (0, q_3) \\ \frac{q_2 q_3}{(q_2 q_3 - q_1 q_3 + q_4 q_1)^2} & (x - q_4) & x \in (q_3, q_4) \end{cases} , \tag{12}$$

and

$$s_3(x, \mathbf{q}) = \begin{cases} \frac{q_2(q_1 - q_2)}{(q_2 q_3 - q_1 q_3 + q_4 q_1)^2} & x & x \in (0, q_3) \\ \frac{q_1(q_1 - q_2)}{(q_2 q_3 - q_1 q_3 + q_4 q_1)^2} & (x - q_4) & x \in (q_3, q_4). \end{cases} . \tag{13}$$

Similar expressions hold for $s_2(x, \mathbf{q})$ and $s_4(x, \mathbf{q})$.

Remark. It is important to note that the solution $w(x, \mathbf{q})$ has an explicit dependency on all the parameters at **all points** $x \in [0, q_4]$. We shall use these exact solutions to test the results of numerically generated sensitivities. In particular, we use a discontinuous Galerkin finite element method to solve elliptic boundary value problems that are satisfied by the sensitivities $s_i(x, \mathbf{q})$, $i = 1, 2, 3, 4$. These equations are called the sensitivity equations and the process of computing the sensitivities by solving these boundary value problems is called the Continuous Sensitivity Equation Method (C-SEM).

3.1 The Sensitivity Equations

We denote by $'$ the derivative with respect to the state variable x and by $s_i(x, \mathbf{q})$ the derivative of $w(x, \mathbf{q})$ with respect to q_i. Thus, $s_i(x, \mathbf{q}) = \frac{\partial w(x,\mathbf{q})}{\partial q_i}$, $i = 1, 2, 3, 4$. To derive the sensitivity equations, one formally differentiates (6) with respect to the parameter q_i and interchanges the order of differentiation to obtain

$$(k(x, \mathbf{q}) s_i'(x, \mathbf{q}))' = 0 \qquad x \in (0, q_4). \tag{14}$$

It is important to note that at this stage this is a purely formal derivation that will be justified later. In order to obtain the interface and boundary conditions for the sensitivities, one again formally differentiates the corresponding interface and boundary conditions for $w(x, \mathbf{q})$. This process leads to boundary and interface conditions for the four sensitivity functions. In addition to the elliptic equation (14), the sensitivities $s_i(x, \mathbf{q})$, $i = 1, 2, 3, 4$ satisfy specific boundary and interface conditions. For the two sensitivities $s_1(x, \mathbf{q})$ and $s_3(x, \mathbf{q})$ these conditions are

$$\begin{array}{r} s_1(0) = 0 \\ s_1(q_4) = 0 \\ k(x, \mathbf{q}) s_1'(q_3^-) - k(x, \mathbf{q}) s_1'(q_3^+) = -w'(q_3^-) \\ s_1(q_3^-) - s_1(q_3^+) = 0 \end{array}, \tag{15}$$

and

$$\begin{array}{r} s_3(0) = 0 \\ s_3(q_4) = 0 \\ k(x, \mathbf{q}) s_3'(q_3^-) - k(x, \mathbf{q}) s_3'(q_3^+) = 0 \\ s_3(q_3^-) - s_3(q_3^+) = w'(q_3^+) - w'(q_3^-) \end{array}, \tag{16}$$

respectively. Similar conditions hold for $s_2(x, \mathbf{q})$ and $s_4(x, \mathbf{q})$. The conditions for $s_3(x, \mathbf{q})$ were derived in [2]. Also, note that since q_4 is the end point of the interval, the boundary conditions at that point is not zero.

3.2 Variational Formulations of the Sensitivity Equations

In this section we present the variational problems for each sensitivity $s_1(x, \mathbf{q})$ and discuss the well-posedness of this problem. This is the first step in developing accurate and convergent numerical scheme for the sensitivities. A detailed analysis is presented for $s_1(x, \mathbf{q})$ and $s_2(x, \mathbf{q})$ is similar. The derivation of the sensitivity equations for $s_4(x, \mathbf{q})$ and $s_3(x, \mathbf{q})$ may be found in [1] and [2], respectively, and will not be given here. However, it is important to note that the interface location sensitivity $s_3(x, \mathbf{q})$ is not continuous across the interface and this is one of the motivation for the use of discontinuous finite element methods in [2].

In order to develop the appropriate variational (weak) formulation of the sensitivity equation for $s_1(x, \mathbf{q})$ we define $W = \{v \in H_0^1(0, q_4) \quad : \quad kv' \in H^1(0, q_4)\}$ and let

$$a(v, s) = -\langle (kv')', s) \rangle$$

be the "natural" bilinear form on $W \times L^2(0, q_4)$. Here, $\langle \cdot, \cdot \rangle$ is the usual inner product on $L^2(0, q_4)$. The weak formulation for the sensitivity equations (14) with conditions (15)-(16) for s_i can be written as a variational problem of the form: Find $s(x, \mathbf{q}) \in L^2(0, q_4)$ such that

$$a(v, s) = L_i(v), \quad \forall v \in W, \tag{17}$$

where $L_i(v)$ is a linear functional that depends on i and that takes a particular form in each case depending on the boundary and interface conditions (15)-(16).

The properties of the bilinear form $a(\cdot, \cdot)$ can be found in [2]. We focus on the first sensitivity $s_1(x, \mathbf{q})$ and refer the reader to the papers [10], [1] and [2] for the other cases. In the rest of this section we study the solutions of (14) with conditions (15) and those of the weak formulation (17) for $s_1(x, \mathbf{q})$. The following theorem states that (17) is equivalent to the elliptic boundary value problem defined by (14) with conditions (15). Recall that $w(x, \mathbf{q})$ is the solution of (6)-(10).

Theorem 1. *The function* $s_1(x, \mathbf{q}) \in L^2(0, q_4)$ *is the solution of the variational equation*

$$-\langle (kv')', s\rangle = (-\frac{\partial w}{\partial x} v)({q_3}^-) \quad \forall v \in W \tag{18}$$

if and only if it is a solution of (14)-(15). Moreover, $s_1(x, \mathbf{q}) \in H_0^1(0, q_4)$ *is a piecewise linear continuous function.*

Remark. We note that it is possible to show that all the variational problems defined above are well-posed weak equations. The choice of the linear functional L_i for $s_i(x, \mathbf{q})$, $i = 1, 2, 3, 4$ are defined by

$$L_i(v(\cdot)) = \beta_i G_i(v(\cdot)), \tag{19}$$

where

$$\beta_i = \begin{cases} -w'(q_3^-) & i = 1 \\ w'(q_3^+) & i = 2 \\ w'(q_3^+) - w'(q_3^-) & i = 3 \\ \frac{q_1 - q_2}{q_4} w'(q_4) & i = 4 \end{cases} \quad ; \quad G_i(v(\cdot)) = \begin{cases} v(q_3) & i = 1, 2 \\ (\kappa v')(q_3) & i = 3 \\ (\kappa v)(q_3^-) & i = 4 \end{cases} . \tag{20}$$

Complete proofs for these sensitivities and in higher dimension will appear in a forthcoming paper. We turn now to an approximation scheme. The scheme was first proposed in [2]. We show that applying this scheme to the sensitivity equations is highly accurate. In fact, it is possible to obtain error estimates based on the variational formulations such as (18) above.

4 Approximation of the Sensitivity Equations

We use the Petrov-Galerkin finite element scheme presented in [2] to approximate the sensitivity equations defined by the variational equation (14) with boundary and interface conditions (15)-(16). We also use the same scheme to approximate the forward problem defined by (6)-(10).

We briefly described the space containing the trial functions and the one containing the test functions. A more detailed description can be found in [2]. Define the partition $0 = x_0 < x_1 < x_2 < \cdots < x_{N+1} = q_4$, where $q_3 = x_k$ for some integer k, $0 < k \le N$, $h = x_i - x_{i-1}$, and let S_h (the space of trial functions) be a space of functions that are polynomials of degree 1 on $e_i = [x_{i-1}, x_i]$

$$S_h = \{s \in L^2(0, q_4) : s(0) = s(q_4) = 0, s|_{e_i} \in P_1(e_i), i = 1, N+1\}.$$

let $\zeta_i = \frac{x - x_{i-1}}{x_i - x_{i-1}}$ and define

$$\Phi_{2i-1} = \begin{cases} \zeta_i & x \in e_i \\ 0 & \text{otherwise} \end{cases} \quad ; \quad \Phi_{2i} = \begin{cases} 1 - \zeta_{i+1} & x \in e_{i+1} \\ 0 & \text{otherwise} \end{cases} .$$

With this definition it follows that $S_h = span\,\{\Phi_i, i = 1, ..., 2N\}$. The space of test functions

$$V_h = \{v \in W : v(0) = v(1) = v'(0) = v'(q_4) = 0, v|_{e_i} \in P_3(e_i), i = 1, \cdot\cdot N+1\}$$

is spanned by the piecewise cubic functions

$$\Psi_{2i-1} = \begin{cases} \zeta_i^2(3 - 2\zeta_i) & x \in e_i \\ (1 - \zeta_{i+1})^2(2\zeta_{i+1} + 1) & x \in e_{i+1} \\ 0 & \text{otherwise} \end{cases} \quad ; \quad \Psi_{2i} = \begin{cases} h\zeta_i^2(1 - \zeta_i) & x \in e_i \\ h(1 - \zeta_{i+1})^2\zeta_{i+1} & x \in e_{i+1} \\ 0 & \text{otherwise} \end{cases}$$

so that $V_h = span\,\{\Psi_1, \cdot, \cdot, \Psi_{2N}\}$. Note that $\Psi_1, \Psi_2, \Psi_{2N}$ and Ψ_{2N-1} must be modified so as to be in V_h. We also modify Ψ_{2k} when $q_3 = x_k$ in order to admit the jump at q_3, as follows

$$\Psi_{2k} = \begin{cases} h\zeta_k^2(1 - \zeta_k) & x \in e_k \\ Rh(1 - \zeta_{k+1})^2\zeta_{k+1} & x \in e_{k+1} \\ 0 & \text{otherwise} \end{cases} ,$$

where $R = \frac{k(x,\mathbf{q})|_{q_3^-}}{k(x,\mathbf{q})|_{q_3^+}}$. It can be shown that $S_h = span\,\{\Psi_1'', ..., \Psi_{2N}''\}$ (see Lemma 3 in [2]).

Remark. In order to use the same test functions $V_h = \{\Psi_i, \quad i = 1, \cdots, 2N\}$ for $s_i(x, \mathbf{q})$, $i = 1, 2, 3, 4$ and $w(x, \mathbf{q})$, we transform the systems corresponding to $s_4(x, \mathbf{q})$ and $w(x, \mathbf{q})$ in order to satisfy the null condition at q_4. This can be done, in each case, by subtracting a linear function that satisfies the condition at the end point, *i.e.*, $\hat{w}(x) = w(x) - \frac{x}{q_4}$ and $\hat{s_4}(x) = s_4(x) + w'(q_4)\frac{x}{q_4}$. For simplicity we will omit the hat and note these new functions by $s_4(x, \mathbf{q})$ and $w(x, \mathbf{q})$.

The sensitivity functions $s_i(x, \mathbf{q})$, $i = 1, 2, 3, 4$ are approximated by

$$s_{ih} = \sum_{j=1}^{2N} z_{i,j} \Phi_j(x)$$

and the problem of finding s_{ih} reduces to the following finite dimensional problem: Find $s_{ih} \in S_h$, $i = 1, 2, 3, 4$ such that

$$a(\Psi_p, s_{ih}) = L_i(\Psi_p(\cdot)) \qquad p = 1, 2, ..., 2N \tag{21}$$

where L_i is defined by (19)-(20) above. This problem has a unique solution since $a(\Psi_i, s_{l_h}) = 0$ implies $\langle \Psi_p'', k s_h \rangle = 0$, $\forall p = 1, \cdots, 2N$ and $\left\{\Psi_p'', \quad p = 1, \cdots, 2N\right\}$ is a basis for S_h. Equation (21) is equivalent to the linear system defined by

$$\sum_{j=1}^{2N} a(\Psi_p, \Phi_j) z_{i,j} = L_i(\Psi_p(\cdot)) \qquad p = 1, 2, ..., 2N$$

and this system is used to compute the approximate sensitivities.

4.1 Numerical Results

We present numerical results obtained when the actual parameter values are $q_1 = 1$, $q_2 = 2$, $q_3 = .4$ and $q_4 = 1$. The function $w_k(x)$ is calculated with a step of $k = \frac{1}{50}$ and we use this approximation to compute the sensitivity functions $s_{i_{k,h}}$, $i = 1, 2, 3, 4$ with a step of $h = \frac{1}{20}$. The plot of all sensitivities are shown in Figure 1. It can be seen that at the interface point $q_3 = 0.4$, the sensitivities functions change their shape to satisfy the interface conditions. In Table 1 we show the relative errors for different partitions $N = 5, 10, 15, 60$ of $[0, 1]$ and perturbations of 5% and 10% in q_1. Analogous numerical experiments for perturbations on the parameter q_4 are shown in Table 2. The error between the corresponding numerical solutions is now concentrated at the right end of the interval.

N	$\mathbf{q} = (0.90, 2, 0.4, 1)$	$\mathbf{q} = (0.95, 2, 0.4, 1)$	$\mathbf{q} = (1.05, 2, 0.4, 1)$	$\mathbf{q} = (1.10, 2, 0.4, 1)$
$N = 5$	0.0211	0.0103	0.0099	0.0194
$N = 10$	0.0217	0.0106	0.0101	0.0199
$N = 15$	0.0219	0.0107	0.0103	0.0201
$N = 60$	0.0225	0.0110	0.0105	0.0206

Table 1. Relative error of the solutions for perturbations in the parameter $q_1 = 1$.

N	$\mathbf{q} = (1, 2, 0.4, 0.90)$	$\mathbf{q} = (1, 2, 0.4, 0.95)$	$\mathbf{q} = (1, 2, 0.4, 1.05)$	$\mathbf{q} = (1, 2, 0.4, 1.10)$
$N = 5$	0.0791	0.0381	0.0953	0.1159
$N = 10$	0.0768	0.0370	0.0526	0.0714
$N = 15$	0.0760	0.0366	0.0377	0.0714
$N = 60$	0.0765	0.0368	0.0364	0.0687

Table 2. Relative error of the solutions for perturbations in the parameter $q_4 = 1$.

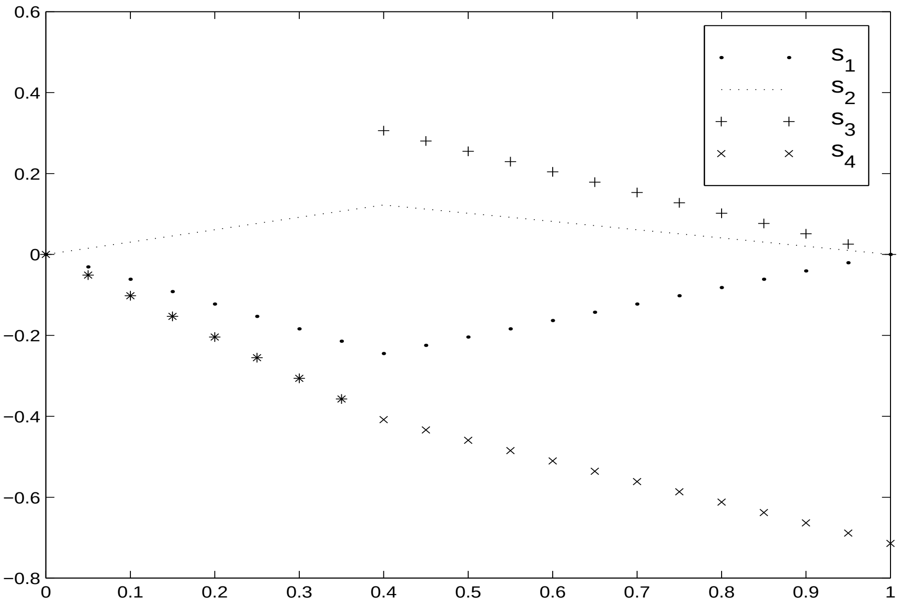

Fig. 1 Sensitivity Functions $s_{l_{k,h}}, l = 1,..,4, k = \frac{q_4}{50}, h = \frac{q_4}{20}$

5 Conclusions

In this short paper we analyzed the sensitivity equations for a 1D elliptic interface problem that is similar to a simplified 1D version of an EEG problem. The equations corresponding to the sensitivity of the solution with respect to the parameters of the problem were stated and its variational form were analyzed. Approximate solutions were calculated by a discontinuous finite element scheme. Typical numerical results were presented to illustrate the method. The 3D inverse problem will be the subject of a future paper.

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