Mathematical Aspects and Numerical Computations of an Inverse Boundary Value Identification Using the Adjoint Method

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Abstract

The purpose of this study is to show some mathematical aspects of the adjoint method that is a numerical method for the Cauchy problem, an inverse boundary value problem. The adjoint method is an iterative method based on the variational formulation, and the steepest descent method minimizes an objective functional derived from our original problem. The conventional adjoint method is time-consuming in numerical computations because of the Armijo criterion, which is used to numerically determine the step size of the steepest descent method. It is important to find explicit conditions for the convergence and the optimal step size. Some theoretical results about the convergence for the numerical method are obtained. Through numerical experiments, it is concluded that our theories are effective.

Key words: adjoint method, boundary value identification, Cauchy problem, convergence proof, optimal step size, steepest descent method, variational formulation

1 Introduction

The Cauchy problem is known as an inverse problem. This problem is to identify unknown boundary value on a part of the boundary of a bounded domain for the given boundary data on the rest of the boundary. In this sense, the problem is regarded as an inverse boundary value problem.

A numerical method for solution of the Cauchy problem, proposed by Onishi et al. [3], is based on the variational formulation. Namely, this method is constructed by formulating the original problem to a minimization problem of a functional. The steepest descent method numerically minimizes the
functional. Finally, the numerical method reduces to an iterative process in which two direct problems are alternately solved. The numerical method is also called the adjoint method, and has been applied to some inverse problems. The effectiveness of the method has been shown by numerical examples [1], [4].

However, mathematical properties of the method have not been clear, yet. Actually, although the step size of the steepest descent method is a very important factor to influence convergence speed, it is difficult to obtain theoretically the suitable step size in general. Hence, in the conventional adjoint method, the step size is numerically determined by the Armijo criterion [5]. But, the Armijo criterion requires many evaluations because we have to solve the direct problem many times. It is a big disadvantage that the conventional method is time-consuming. Moreover, the convergence of this method has not been proved, yet.

In this paper, we will consider an annulus domain for simplicity to prove that the estimated boundary value obtained by the adjoint method converges to the exact one. Moreover, we will obtain the suitable step size such that the convergence becomes more rapid. We will confirm the effectiveness of some theoretical results through simple numerical experiments using the finite element method.

2 Problem Setting

For a two dimensional annulus domain \( \Omega := \{ (x, y) ; R_{id}^2 < x^2 + y^2 < R_d^2 \} \) with the outer boundary \( \Gamma_d := \{ (x, y) ; x^2 + y^2 = R_d^2 \} \) and the inner one \( \Gamma_{id} := \{ (x, y) ; x^2 + y^2 = R_{id}^2 \} \), we consider the Cauchy problem of the Laplace equation:

**Problem 1** For given Cauchy data \((\pi, \eta) \in H^{1/2}(\Gamma_d) \times \{ \partial v/\partial n \in H^{-1/2}(\Gamma_d) \}; \)

\[-\Delta v = 0 \text{ in } \Omega, \quad v|_{\Gamma_d} = \pi, \quad v|_{\Gamma_{id}} = \omega, \quad \omega \in H^{1/2}(\Gamma_{id}) \}, \]

find \( u \in H^{1/2}(\Gamma_d) \) such that

\[
\begin{cases}
-\Delta u = 0 & \text{in } \Omega, \\
u = \pi, & \frac{\partial u}{\partial n} = \eta & \text{on } \Gamma_d,
\end{cases}
\]

where \( n \) denotes the unit outward normal to \( \Gamma_d \).

In engineering and medical science, this is an important problem known as a mathematical model of the inverse problem of the electrocardiography, which is a problem to identify unknown electric potential on the surface of a human heart by observing the electric potential on the surface of a human body.
3 Variational Formulation

To solve Problem 1, we consider the following variational problem based on the method of the least squares:

**Problem 2** Find $\omega^* \in H^{1/2}(\Gamma_{id})$ such that

$$J(\omega^*) = \inf_{\omega \in H^{1/2}(\Gamma_{id})} J(\omega), \quad (1)$$

where the functional $J$ is defined as

$$J(\omega) := \int_{\Gamma_d} |v(\omega) - \overline{u}|^2 d\Gamma,$$

and $v = v(\omega) \in H^1(\Omega)$ depending on the given boundary value $\omega \in H^{1/2}(\Gamma_{id})$ is the solution of the following mixed boundary value problem called the primary problem:

$$\begin{align*}
-\Delta v &= 0 \quad \text{in} \quad \Omega, \\
\frac{\partial v}{\partial n} &= \overline{q} \quad \text{on} \quad \Gamma_d, \\
v &= \omega \quad \text{on} \quad \Gamma_{id}.
\end{align*} \quad (2)$$

Our strategy is to find the minimum of $J$ by generating a minimizing sequence \(\{\omega_k\}_{k=0}^\infty \subset H^{1/2}(\Gamma_{id})\) by the steepest descent method:

$$\omega_{k+1} = \omega_k - \rho_k J'(\omega_k), \quad (3)$$

starting with an initial guess $\omega_0 \in H^{1/2}(\Gamma_{id})$, with a suitably chosen step size \(\{\rho_k\}_{k=0}^\infty\). The derivative $J'(\omega)$ is the first variation of $J$, defined by

$$J(\omega + \delta \omega) - J(\omega) = (J'(\omega), \delta \omega) + o(\|\delta \omega\|),$$
where $(\cdot, \cdot)$ and $\| \cdot \|$ denote the inner product and the norm in $L^2(\Gamma_{id})$, respectively:
\[
(f, g) := \int_{\Gamma_{id}} fg d\Gamma, \quad \|f\| := (f, f)^{1/2}.
\]

The first variation is explicitly given \cite{1}, \cite{3} -- \cite{5} by
\[
J'(\omega) = -\frac{\partial \hat{v}}{\partial n}|_{\Gamma_{id}},
\]
where $\hat{v} = \hat{v}(v(\omega)) \in H^2(\Omega)$ depending on the solution $v = v(\omega)$ of the primary problem is the solution of the following mixed boundary value problem called the adjoint problem:
\[
\begin{cases}
-\Delta \hat{v} = 0 & \text{in } \Omega, \\
\frac{\partial \hat{v}}{\partial n} = 2(v - \bar{u}) & \text{on } \Gamma_d, \\
\hat{v} = 0 & \text{on } \Gamma_{id}.
\end{cases}
\]

We remark that $J'(\omega) \in H^{1/2}(\Gamma_{id})$.

4 Algorithm

Our numerical method for the Cauchy problem reduces to an iterative process to minimize the functional (1) by the steepest descent method (3) after solving the primary problem (2) and the adjoint problem (5) to obtain the first variation (4).

For given $\omega = \omega_k$, we denote the solutions of the primary and the adjoint problems by $v_k := v(\omega_k)$, $\hat{v}_k := \hat{v}(v(\omega_k))$, respectively. Then, our algorithm can be summarized as follows:

Algorithm

**Step 0.** Pick an initial guess $\omega_0 \in H^{1/2}(\Gamma_{id})$, and set $k := 0$.

**Step 1.** Solve the primary problem
\[
\begin{cases}
-\Delta v_k = 0 & \text{in } \Omega, \\
\frac{\partial v_k}{\partial n} = \bar{q} & \text{on } \Gamma_d, \\
v_k = \omega_k & \text{on } \Gamma_{id}
\end{cases}
\]

to find $v_k|_{\Gamma_d} \in H^{1/2}(\Gamma_d)$. 

4
Step 2. Solve the adjoint problem

\[
\begin{align*}
-\Delta \hat{v}_k &= 0 \quad \text{in } \Omega, \\
\frac{\partial \hat{v}_k}{\partial n} &= 2(v_k - \overline{u}) \quad \text{on } \Gamma_d, \\
\hat{v}_k &= 0 \quad \text{on } \Gamma_{id}
\end{align*}
\]  

(7)

to find the first variation

\[J'(\omega_k) = -\frac{\partial \hat{v}_k}{\partial n}_{\Gamma_{id}} \in H^{1/2}(\Gamma_{id}).\]

Step 3. Choose the step size \( \rho_k \).

Step 4. Update the boundary value by the steepest descent method

\[\omega_{k+1} = \omega_k - \rho_k J'(\omega_k).\]  

(8)

Step 5. Set \( k := k + 1 \), and go to Step 1.

In numerical computations, the primary and the adjoint problems in Steps 1 and 2 are numerically solved by the triangular finite element method. The conventional method to choose the suitable step size \( \rho_k \) in Step 3 is the Armijo criterion, which guarantees for the sequence \( \{\rho_k\}_{k=0}^\infty \) to satisfy

\[J(\omega_k - \rho_k J'(\omega_k)) \leq J(\omega_k) - \xi \rho_k \|J'(\omega_k)\|^2\]  

(9)

with a constant \( 0 < \xi < 1/2 \).

Controlling the step size

Step 3.0. Give \( 0 < \xi < 1/2, \ 0 < \tau < 1 \) and the sufficiently small \( \varepsilon > 0 \).

Step 3.1. If \( \|J'(\omega_k)\| < \varepsilon \), then stop; else go to Step 3.2.

Step 3.2. Set \( \beta_0 := 1, \ m := 0 \).

Step 3.3. If \( J(\omega_k - \beta_m J'(\omega_k)) \leq J(\omega_k) - \xi \beta_m \|J'(\omega_k)\|^2 \), then set \( \rho_k := \beta_m \); else go to Step 3.4.

Step 3.4. Set \( \beta_{m+1} := \tau \beta_m \).

Step 3.5. Set \( m := m + 1 \), and go to Step 3.3.

To choose the step size, we have to evaluate the functional value on the left hand side in (9) many times. It means that the primary problem has to be solved many times. This is an disadvantage of the conventional method.

5 Convergence Proof and the Optimal Step Size

In this section, we prove that our numerical method is convergent under some assumption. Moreover, we propose suitable step sizes to avoid the disadvan-
tage of the conventional method. The following argument is based on the convergence proof of the Dirichlet-Neumann alternating method [6], which is one of the domain decomposition methods [2].

We denote by $v^*$ and $\hat{v}^*$ the solutions of the primary and the adjoint problems for the boundary value $\omega = \omega^*$, respectively. Let the error functions $e_k := v^* - v_k$, $\hat{e}_k := \hat{v}^* - \hat{v}_k$, and $\mu_k := \omega^* - \omega_k$. Then, from (6) and (7), we see that the functions $e_k$ and $\hat{e}_k$ are the solutions of

$$
\begin{cases}
-\Delta e_k = 0 & \text{in } \Omega, \\
\frac{\partial e_k}{\partial n} = 0 & \text{on } \Gamma_d, \\
e_k = \mu_k & \text{on } \Gamma_{id},
\end{cases}
$$

and

$$
\begin{cases}
-\Delta \hat{e}_k = 0 & \text{in } \Omega, \\
\frac{\partial \hat{e}_k}{\partial n} = 2e_k & \text{on } \Gamma_d, \\
\hat{e}_k = 0 & \text{on } \Gamma_{id},
\end{cases}
$$

respectively.

We assume that the error $\mu_k$ can be expanded into the finite Fourier series:

$$
\mu_k = \sum_{|j|=M}^{N} a_j^{(k)} e^{ij\theta}
$$

with some integers $M$ and $N$ such that $N \geq M \geq 0$. From (10), we have

$$
e_k|_{\Gamma_d} = \sum_{|j|=M}^{N} \frac{2R_d |j| R_{id} |j|}{R_d 2|j| + R_{id} 2|j|} a_j^{(k)} e^{ij\theta}.
$$

Substituting (13) into (11), we can derive

$$
\frac{\partial \hat{e}_k}{\partial n} \bigg|_{\Gamma_{id}} = - \sum_{|j|=M}^{N} \frac{8R_d 2|j| + R_{id} 2|j|}{(R_{id} 2|j| + R_d 2|j|)^2} a_j e^{ij\theta}.
$$

Here, noting that $\hat{v}^* = 0$, we have

$$
J'(\omega_k) = \frac{\partial \hat{\varepsilon}_k}{\partial n} \bigg|_{\Gamma_{id}}.
$$

We can see from (8) that

$$
\mu_{k+1} = \mu_k + \rho_k J'(\omega_k).
$$

Substituting (12) and (15) (namely (14)) into (16), we have

$$
a_j^{(k+1)} = (1 - C_j \rho_k) a_j^{(k)}
$$
with
\[ C_j := \frac{8R_d^{2|j|+1}R_{id}^{2|j|-1}}{(R_{id}^{2|j|} + R_d^{2|j|})^2}. \]

If we take the step size as
\[ 0 < \rho_k < \frac{2}{C_M}, \]
then we have
\[ |\delta_j^{(k)}| \leq \delta^{(k)} = \max \{|1 - C_M \rho_k|, |1 - C_N \rho_k|\} < 1 \quad (18) \]
with \( \delta_j^{(k)} := 1 - C_j \rho_k \) and \( \delta^{(k)} := \max_{M \leq j \leq N} |\delta_j^{(k)}| \). It follows that \( \{\|\mu_k\|\}_{k=0}^{\infty} \) is a strictly monotone decreasing sequence:
\[ \|\mu_{k+1}\| \leq \delta^{(k)}\|\mu_k\| \]
with the compression factor \( \delta^{(k)} < 1 \). Therefore, we obtain that \( \mu_k \rightarrow 0 \), that is, \( \omega_k \rightarrow \omega^* \) as \( k \rightarrow \infty \).

We notice that the convergence cannot be guaranteed in general because \( \delta^{(k)} = 1 \) in (18) if \( \mu_k \) is expanded into the infinite series.

As a consequence, we can obtain the following theorem:

**Theorem 1** For the exact boundary value \( \omega^* \), we assume that the error \( \mu_k = \omega^* - \omega_k \) can be expanded into the finite Fourier series:
\[ \mu_k = \sum_{|j|=M}^{N} a_j^{(k)} e^{ij\theta} \quad (19) \]
with some integers \( M \) and \( N \) such that \( N \geq M \geq 0 \). If we take the step size as
\[ 0 < \rho_k < \frac{2}{C_M}, \quad C_j := \frac{8R_d^{2|j|+1}R_{id}^{2|j|-1}}{(R_{id}^{2|j|} + R_d^{2|j|})^2}, \]
then \( \{\omega_k\}_{k=0}^{\infty} \) converges to \( \omega^* \).

**Corollary 1** The optimal step size \( \rho_{opt} \) in the sense that the compression factor is minimized is given by
\[ \rho_{opt} = \frac{2}{C_M + C_N}. \quad (20) \]
Then, the optimal compression factor \( \delta_{opt} \) is given by
\[ \delta_{opt} = \frac{C_M - C_N}{C_M + C_N}. \quad (21) \]
Proof Taking
\[|1 - C_M \rho_k| = |1 - C_N \rho_k| = \delta_{\text{opt}}\]
so as to minimize \(\delta^{(k)}\) in (18), we obtain (20) and (21). □

The next theorem is very effective in actual computations.

**Theorem 2** The error \(\mu_k\) is assumed to be expanded into (19). If we put \(\rho_k = 1/C_{M+k}\) or \(\rho_k = 1/C_{N-k}\) \((k = 0, 1, \ldots, N - M)\), then we have \(\mu_{N-M+1} = 0\), namely the exact \(\omega^*\) is obtained after \((N - M + 1)\) iterations.

Proof For \(k = 0, 1, \ldots, N - M\), substituting \(\rho_k = 1/C_{M+k}\) (resp. \(\rho_k = 1/C_{N-k}\)) into (17), we have \(a_{M+k}^{(k+1)} = 0\) (resp. \(a_{N-k}^{(k+1)} = 0\)). Then, it follows that \(a_{M+k}^{(l)} = 0\) (resp. \(a_{N-k}^{(l)} = 0\)) for all \(l = k + 1, k + 2, \ldots, N - M + 1\). □

6 Numerical Experiments

Let the radii \(R_d = 3\) and \(R_{id} = 1\). The domain \(\Omega\) is divided into triangular finite elements with 8552 elements and 4436 nodes. We take \(\omega_0 = 0\) as an initial guess. The stop condition of our calculations is given by \(J(\omega_k) < 10^{-5}\).

![Fig. 2. Functional values](image)

As the first example, let the Cauchy data be \((\pi, \varphi) = (9 \cos 2\theta, 6 \cos 2\theta)\). Then, the exact potential in \(\Omega\) and the related exact boundary value on \(\Gamma_{id}\) can be written as follows:

\[
\begin{align*}
\{ & u^* = r^2 \cos 2\theta, \\
& \omega^* = u^*|_{\Gamma_{id}} = \cos 2\theta 
\end{align*}
\]

We can see from the Cauchy data that \(M = N = 2\). It follows that \(\rho_{\text{opt}} = 1/C_2 = 1681/486(\approx 3.46)\) and \(\delta_{\text{opt}} = 0\). Hence, theoretically it should hold that \(\omega_1 = \omega^*\). But, in actual computations, we remark that \(\omega_1 \neq \omega^*\) due to discretization errors by the finite element method. For \(k \geq 1\), we regard that

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$M = 0$ and $N$ is sufficiently large. Then, according to Corollary 1, we have $\rho_{\text{opt}} \approx 2/C_0 = R_{\text{id}}/R_d = 1/3$. Hence, we take

$$\rho_k = \begin{cases} 
1681/486(\approx 3.46) & (k = 0), \\
1/3(\approx 0.33) & (k \geq 1)
\end{cases} \quad (22)$$

Then, the graph (a) in Figure 2 shows the variations of functional value. Since the functional value decreases steeply by taking the step sizes as large as possible, the convergence becomes rapid. On the other hand, the graph (b) is the result in the case when we apply the Armijo criterion with $\xi = 1/3$ and $\tau = 1/2$. When the Armijo criterion is applied, only to choose the step sizes, the primary problem has to be solved 89 times. Hence, until the estimated boundary value converges, in all we have to solve the direct problems 58 (= 29 $\times$ 2) times in the case of the graph (a) and 163 (= 37 $\times$ 2 $+$ 89) times in the case of the graph (b), respectively. We can see that (22) makes convergence more rapid than the Armijo criterion. On the other hand, Figure 3 shows the estimated boundary value $\omega_k$ and the exact one $\omega^*$. We can see that $\omega_1$ is in good agreement with $\omega^*$. It is concluded that the estimated boundary value quickly converges to the exact one.

As the second example, we assume that the Cauchy data is

$$(\pi, \mathcal{J}) = \left( 6 \sin \theta - \frac{3}{2} \cos \theta + \frac{9}{4} \cos 2\theta, 2 \sin \theta - \frac{1}{2} \cos \theta + \frac{3}{2} \cos 2\theta \right).$$

Then, the exact potential in $\Omega$ and the related exact boundary value on $\Gamma_{\text{id}}$ can be written as follows:

$$\begin{cases} 
\omega^* = u|_{\Gamma_{\text{id}}} = 2 \sin \theta - \frac{1}{2} \cos \theta + \frac{1}{4} \cos 2\theta.
\end{cases}$$
We can see from the Cauchy data that $M = 1$ and $N = 2$. But, due to numerical errors, we assume that $M = 0$. According to Theorem 2, we take the step size as

$$\rho_k = \begin{cases} 
1/C_{2-k} & (k = 0, 1, 2) \\
1/3(\approx 0.33) & (k \geq 3)
\end{cases} \quad (23)$$

Then, the graph (c) in Figure 4 shows the variations of functional value. As we can see, the functional value reaches less than $10^{-5}$ at $k = 5$. On the other hand, using the Armijo criterion with $\xi = 1/3$ and $\tau = 1/2$, we obtain the functional value less than $10^{-5}$ at $k = 31$, which is shown as the graph (a). When we apply the Armijo criterion, only to choose the step sizes, the primary problem has to be solved 76 times. Hence, until the estimated boundary value converges, in all we have to solve the direct problems $10(= 5 \times 2)$ times in the case of the graph (c) and $138(= 31 \times 2 + 76)$ times in the case of the graph (a), respectively. If we do not know the concrete values of $M$ and $N$, it is reasonable to assume that $M = 0$ and $N$ is sufficiently large. Then, the step size is taken as $\rho_k = 1/3(\approx 0.33)$ for all $k \geq 0$ according to Corollary 1. The variations of functional value for this step size are shown by the graph (b). Although the number of iterations for the graph (b) is greater than that for the graph (a), the computational cost for (b) is less than that for (a) in all.

Figure 5 shows the estimated boundary value $\omega_k$ and the exact one $\omega^*$. We can see that $\omega_2$ is roughly the same as $\omega^*$.

Therefore, through two examples, it is concluded that the computational cost can reduce and the estimated boundary value quickly converges to the exact one by applying Corollary 1 and Theorem 2, which are very effective in numerical computations.
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