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ELLIPTIC INVERSE PROBLEMS OF IDENTIFYING NONLINEAR PARAMETERS

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Dedicated to Stephen M. Robinson on his 75th birthday

ABSTRACT. Inverse problems of identifying parameters in partial differential equations (PDEs) is an important class of problems with many real-world applications. Inverse problems are commonly studied in optimization setting with various known approaches having their advantages and disadvantages. Although a non-convex output least-squares (OLS) objective has often been used, a convex modified output least-squares (MOLS) attracted quite an attention in recent years. However, the convexity of the MOLS has only been established for parameters appearing linearly in the PDEs. The primary objective of this work is to introduce and analyze a variant of the MOLS for the inverse problem of identifying parameters that appear nonlinearly in variational problems. Besides giving an existence result for the inverse problem, we derive the first-order and second-order derivative formulas for the new functional and use them to identify the conditions under which the new functional is convex. We give a discretization scheme for the continuous inverse problem and prove its convergence. We also obtain discrete formulas for the new MOLS functional, and present detailed numerical examples.

1. INTRODUCTION

Applied models frequently lead to partial differential equations involving parameters attributed to physical characteristics of the model. The direct problem in this setting is to solve the partial differential equation. By contrast, an inverse problem seeks for the identification of the parameters when a measurement of a solution of the partial differential equation is available.

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For clarification, consider the boundary value problem (BVP)

$$-\nabla \cdot (q\nabla u) = f \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \partial\Omega, \tag{1.1}$$

where Ω is a sufficiently smooth domain in $\mathbb{R}^2$ or $\mathbb{R}^3$ and $\partial\Omega$ is its boundary. The above BVP models interesting real-world problems and has been studied in great detail. For instance, here $u = u(x)$ may represent the steady-state temperature at a given point x of a body; then q would be a variable thermal conductivity coefficient, and f the external heat source. This system also models underground steady state aquifers in which the parameter q is the aquifer transmissivity coefficient, u is the hydraulic head, and f is the recharge. The inverse problem in the context of the above BVP is to estimate the coefficient q from a measurement z of the solution u.

A number of methods to the aforementioned inverse problem have been proposed in the literature; most involve either regarding (1.1) as a hyperbolic PDE in q or posing an optimization problem whose solution is an estimate of q. The approach of reformulating (1.1) as an optimization problem is divided into two possibilities, namely either formulating the problem as an unconstrained optimization problem or treating it as a constrained optimization problem, in which the PDE itself is the constraint. Among the optimization-based techniques the output least-squares (OLS) method is among the most widely used methods. The output least-squares approach minimizes the functional

$$q \to \|u(q) - z\|^2, \tag{1.2}$$

where z is the data and $u(q)$ solves the variational form of (1.1) given by

$$\int_\Omega q\nabla u \cdot \nabla v = \int_\Omega fv, \quad \text{for all}\, v \in H_0^1(\Omega). \tag{1.3}$$

A known deficiency of the OLS functional is that it is, in general, nonconvex.

There are other functionals that have been used. For example, the equation error method (cf. [1, 2]), consists of minimizing the functional

$$q \to \|\nabla(q\nabla z) + f\|^2_{H^{-1}(\Omega)}$$

where $H^{-1}(\Omega)$ is the dual of $H_0^1(\Omega)$ and z is the data. Chen and Zou [6] developed an augmented Lagrangian algorithm to solve the OLS problem by treating the PDE as an explicit constraint.

Knowles [13] proposed minimizing a coefficient-dependent norm

$$q \to \int q\nabla(u(q) - z) \cdot \nabla(u(q) - z), \tag{1.4}$$

where z is the data and $u(a)$ solves (1.3). Knowles [13] established that the above functional is convex. Some related developments are given in [4, 5, 7, 14].

It is convenient to investigate the inverse problem of parameter identification in an abstract setting allowing for more general PDEs. Let B be a Banach space and let A be a nonempty, closed, and convex subset of B. Given a Hilbert space V, let $T : B \times V \times V \to \mathbb{R}$ be a trilinear form with $T(a, u, v)$ symmetric in u, v, and let m be a bounded linear functional on V. Assume there are constants $\alpha > 0$ and $\beta > 0$

such that the following conditions hold:

$$T(a,u,v) \leq \beta\|a\|_B\|u\|_V\|v\|_V, \quad \text{for all } u,v \in V,\ a \in B, \tag{1.5}$$

$$T(a,u,u) \geq \alpha\|u\|_V^2, \ \text{for all } u \in V,\ a \in A. \tag{1.6}$$

Consider the variational problem: Given $a \in A$, find $u = u(a) \in V$ with

$$T(a,u,v) = m(v), \quad \text{for every } v \in V. \tag{1.7}$$

Due to the imposed conditions, it follows from the Riesz representation theorem that for every $a \in A$, the variational problem (1.7) admits a unique solution $u(a)$. In this abstract setting, the inverse problem of identifying parameter now seeks a in (1.7) from a measurement z of u.

In [10], the following modified OLS functional (MOLS) was introduced

$$J(a) = \frac{1}{2}T(a, u(a)-z, u(a)-z) \tag{1.8}$$

where z is the data (the measurement of u) and $u(a)$ solves (1.7). This functional generalizes (1.4). In [10], the author established that (1.8) is convex and used it to estimate the Lamé moduli in the equations of isotropic elasticity. Studies related to MOLS functional and its extensions can be found in [8, 11, 12].

The first observation necessary for the convexity of the MOLS is that for each a in the interior of A, the first derivative $\delta u = Du(a)\delta a$ is the unique solution of the variational equation (see [10]):

$$T(a,\delta u,v) = -T(\delta a,u,v), \quad \text{for every } v \in V, \tag{1.9}$$

Using (1.9), the authors in [10] obtained the following derivative formulae:

$$DJ(a)\delta a = -\frac{1}{2}T(\delta a, u(a)+z, u(a)-z), \tag{1.10}$$

$$D^2J(a)(\delta a,\delta a) = T(a, Du(a)\delta a, Du(a)\delta a). \tag{1.11}$$

Due to the coercivity (1.6), it follows that $D^2J(a)(\delta a,\delta a) \geq \alpha\|Du(a)\delta a\|_V^2$, and hence the convexity of (1.8) in the interior of A follows.

A careful look at the proofs of the above mentioned results reveals that for the convexity of the MOLS, it is essential that the first argument of T be the parameter to be identified. On the other hand, interesting applications lead to cases when the first argument of T is in fact contains a nonlinear function of the sought parameter (see [15]).

The objective of this paper is to introduce and analyze a variant of the MOLS for the inverse problem of identifying parameter that appears nonlinearly in general variational problems. We are interested in understanding what geometric properties of the MOLS can be retained for such a case. We derive the first-order and second-order derivative formulas for the new functional and use them to identify the conditions under which the new functional is convex. We give a discretization scheme for the continuous inverse problem and prove its convergence. We obtain discrete formulas for the new MOLS functional. We also provide numerical results to show the feasibility of the proposed functional.

2. Solvability of the inverse problem and derivative formulae

Given an open and convex set $S \subset X$, a map $f : S \subset X \to Y$ is directionally differentiable at $x \in S$ in a direction $\delta x \in X$ if the following limit exists

$$f'(x; \delta x) = \lim_{t \downarrow 0} \frac{f(x + t\delta x) - f(x)}{t}.$$

The map f is called directionally differentiable at x if f is directionally differentiable at $x \in S$ in every direction $\delta x \in X$. Given f is directionally differentiable, the second-order directional derivative along directions $(\delta x_1, \delta x_2) \in X \times X$ is given by the limit (provided that it exists):

$$f''(x; \delta x_1, \delta x_2) = \lim_{t \downarrow 0} \frac{f'(x + t\delta x_2; \delta x_1) - f'(x; \delta x_1)}{t}$$

Note that

$$\begin{aligned} Df(x)(\delta x) &= f'(x; \delta x), \\ D^2 f(x)(\delta x_1, \delta x_2) &= f''(x; \delta x_1, \delta x_2) \end{aligned}$$

if f is differentiable, twice differentiable at x, respectively.

Let $\sigma : S \subset B \to B$ be a map such $\sigma(x) \in A$ for every $x \in \mathrm{dom}(\sigma)$. Moreover, assume that σ is continuous and directionally differentiable at any point in the interior of A which we assume to be nonempty. Given $a \in A$, consider the variational problem of finding $u(a) \in V$ such that

$$T(\sigma(a), u(a), v) = m(v), \quad \text{for every } v \in V. \tag{2.1}$$

Our objective is to identify the parameter a from a measurement z of u.

We give the following continuity result for its later use.

Lemma 2.1. *The following bounds are valid:*

$$\|u(a) - u(b)\|_V \le \min\left\{ \frac{\beta}{\alpha}\|u(a)\|_V, \frac{\beta}{\alpha}\|u(b)\|_V, \frac{\beta}{\alpha^2}\|m\|_{V^*} \right\} \|\sigma(b) - \sigma(a)\|_B.$$

Proof. For any $v \in V$, we have $T(\sigma(a), u(a), v) = m(v) = T(\sigma(b), u(b), v)$ implying $T(\sigma(a), u(a), v) - T(\sigma(b), u(b), v) = 0$ or $T(\sigma(a), u(a) - u(b), u(a) - u(b)) = -T(\sigma(a) - \sigma(b), u(b), u(a) - u(b))$. Using (1.5) and (1.6), we get

$$\|u(a) - u(b)\|_V \le \frac{\beta}{\alpha}\|u(b)\|_V \|\sigma(a) - \sigma(b)\|_B,$$

proving the second bound; the first is obtained by interchanging the roles of a and b. The bound $\|u(b)\|_V \le \alpha^{-1}\|m\|_{V^*}$, which is easy to prove, yield the third bound. $\square$

We introduce the following new modified output least squares

$$J(a) = \frac{1}{2} T(\sigma(a), u(a) - z, u(a) - z), \tag{2.2}$$

where z is the data (the measurement of u) and $u(a)$ solves (2.1).

We can now formulate the inverse problem as an optimization problem using (2.2). However, due to the known ill-posedness of inverse problems, we need some kind of regularization for developing a stable computational framework. Therefore, instead of (2.2), we will use its regularized analogue and consider the regularized optimization problem: Find $a \in A$ by solving

$$\min_{a \in A} J_\kappa(a) := \frac{1}{2} T(\sigma(a), u(a) - z, u(a) - z) + \kappa \|a\|_H^2, \tag{2.3}$$

where, given a Hilbert space H, $\kappa > 0$ is a regularization parameter, $u(a)$ is the unique solution of (2.1) for the coefficient a, and z is the measured data.

The following is an existence result for the regularized problem (2.3).

Theorem 2.2. *Assume that the space H is compactly embedded into B, $A \subset H$ is nonempty, closed, and convex. Then* (2.3) *has a nonempty solution set.*

Proof. Since $J_\kappa(a) \geq 0$, for all $a \in A$, there exists a minimizing sequence $\{a_n\}$ in A such that $\lim_{n\to\infty} J_\kappa(a_n) = \inf\{J_\kappa(a) | \, a \in A\}$. Therefore, $\{J_\kappa(a_n)\}$ is bounded from above which implies that $\{a_n\}$ is bounded in H. Due to the compact embedding of H into B, there exists a subsequence converging strongly in B. By keeping the same notations for subsequences as well, we assume that a_n converges strongly some $\bar{a} \in A$. Moreover, due to the continuity of σ, we have $\sigma(a_n) \to \sigma(\bar{a})$. By the definition of u_n, for every $v \in V$, we have $T(\sigma(a_n), u_n, v) = m(v)$, which for $v = u_n$ yields $T(\sigma(a_n), u_n, u_n) = m(u_n)$. Using (1.6), we get $\alpha \|u_n\|_V^2 \leq \|m\|_{V^*} \|u_n\|_V$, which ensures the boundedness of $u_n = u(a_n)$. Therefore, there exists a subsequence of $\{u_n\}$ that converges weakly to some $\bar{u} \in V$. We claim that $\bar{u} = u(\bar{a})$. Recall that for every $v \in V$, we have $T(\sigma(a_n), u_n, v) = m(v)$. This, after a simple rearrangements of terms, implies that $T(\sigma(\bar{a}), \bar{u}, v) - m(v) = -T(\sigma(a_n) - \sigma(\bar{a}), u_n, v) - T(\sigma(\bar{a}), u_n - u, v)$, which, when passed to the limit $n \to \infty$, implies that $T(\sigma(\bar{a}), \bar{u}, v) = m(v)$ as all the terms on the right-hand side go to zero. Since $v \in V$ is arbitrary and since (1.7) is uniquely solvable, we deduce that $\bar{u} = u(\bar{a})$.

We claim that $J(a_n) \to J(\bar{a})$. The identities $T(\sigma(a_n), u_n - z, u_n - z) = m(u_n - z) - T(\sigma(a_n), z, u_n - z)$ and $T(\sigma(\bar{a}), \bar{u} - z, \bar{u} - z) = m(\bar{u} - z) - T(\sigma(\bar{a}), z, \bar{u} - z)$, in view of the rearrangement

$$\begin{aligned} T(\sigma(a_n), z, u_n - z) - T(\sigma(\bar{a}), z, \bar{u} - z) = T(\sigma(a_n) - \sigma(\bar{a}), z, u_n - z) \\ - T(\sigma(\bar{a}), z, u_n - \bar{u}), \end{aligned}$$

ensure that $T(\sigma(a_n), u_n - z, u_n - z) \to T(\sigma(\bar{a}), \bar{u} - z, \bar{u} - z)$, and consequently,

$$\begin{aligned} J_\kappa(\bar{a}) &= T(\sigma(\bar{a}), \bar{u} - z, \bar{u} - z) + \kappa \|\bar{a}\|_H^2 \\ &\leq \lim_{n\to\infty} T(\sigma(a_n), u(a_n) - z, u(a_n) - z) + \liminf_{n\to\infty} \kappa \|a_n\|_H^2 \\ &\leq \liminf_{n\to\infty} \{T(\sigma(a_n), u(a_n) - z, u(a_n) - z) + \kappa \|a_n\|_H^2\} \\ &= \inf\{J_\kappa(a) \, : \, a \in A\}, \end{aligned}$$

confirming that $\bar{a}$ is a solution of (2.3). The proof is complete. ☐

The following result shows the smoothness of the parameter-to-solution map $u : a \to u(a)$. Recall that we are assuming that σ is directionally differentiable.

Theorem 2.3. *For each a in the interior of A, the parameter-to-solution $u : A \subset B \to V$ is directionally differentiable. Moreover, for each direction $\delta a \in B$ the directional derivative $u'(a;\delta a)$ is the unique solution of the following variational equation*

$$T\left(\sigma(a), u'(a;\delta a), v\right) = -T\left(\sigma'(a;\delta a), u(a), v\right), \quad \text{for every } v \in V. \tag{2.4}$$

Furthermore, if σ is differentiable at a, then u is differentiable at a.

Proof. The Lax-Milgram lemma confirms that the variational equation is uniquely solvable. For any a in the interior of A, let $\delta a \in B$ be arbitrary. For any $t > 0$ and any $v \in V$, we have

$$\begin{aligned} T(\sigma(a+t\delta a), u(a+t\delta a), v) &= m(v), \\ T(\sigma(a), u(a), v) &= m(v)\ . \end{aligned}$$

The above equations after a rearrangement of terms, yield

$$\begin{aligned} 0 &= \frac{1}{t}\left[T(\sigma(a+t\delta a), u(a+t\delta a), v) - T(\sigma(a), u(a), v)\right] \\ &= \frac{1}{t}\left[T(\sigma(a+t\delta a), u(a+t\delta a), v) - T(\sigma(a), u(a+t\delta a), v)\right] \\ &+ \frac{1}{t}\left[T(\sigma(a), u(a+t\delta a), v) - T(\sigma(a), u(a), v)\right] \\ &= T\left(\frac{\sigma(a+t\delta a)-\sigma(a)}{t}, u(a+t\delta a), v\right) \\ &+ T\left(\sigma(a), \frac{u(a+t\delta a)-u(a)}{t}, v\right), \end{aligned}$$

and therefore, for an arbitrary $v \in V$, we have

$$T\left(\sigma(a), \frac{u(a+t\delta a)-u(a)}{t}, v\right) = -T\left(\frac{\sigma(a+t\delta a)-\sigma(a)}{t}, u(a+t\delta a), v\right). \tag{2.5}$$

Let $w \in V$ be the unique solution to the following variational equation

$$T\left(\sigma(a), w, v\right) = -T\left(\sigma'(a;\delta a), u(a), v\right), \quad \text{for every } v \in V. \tag{2.6}$$

By combining (2.5) and (2.6), and setting

$$\delta u_t := t^{-1}(u(a+t\delta a) - u(a)),$$

we have

$$\begin{aligned} T\left(\sigma(a), \delta u_t - w, v\right) = &- T\left(\frac{\sigma(a+t\delta a)-\sigma(a)}{t} - \sigma'(a;\delta a), u(a+t\delta a), v\right) \\ &- T\left(\sigma'(a;\delta a), u(a+t\delta a) - u(a), v\right). \end{aligned} \tag{2.7}$$

Taking $v = \delta u_t - w$ in this expression, we get

$$\begin{aligned}\alpha \|\delta u_t - w\|_V^2 &\le T(\sigma(a), \delta u_t - w, \delta u_t - w) \\ &= -T\left(\frac{\sigma(a+t\delta a) - \sigma(a)}{t} - \sigma'(a;\delta a), u(a+t\delta a), \delta u_t - w\right) \\ &\quad - T\big(\sigma'(a;\delta a), u(a+t\delta a) - u(a), \delta u_t - w\big)\end{aligned}$$

and hence

$$\begin{aligned}\alpha \|\delta u_t - w\|_V \le \beta &\left\| \frac{\sigma(a+t\delta a) - \sigma(a)}{t} - \sigma'(a;\delta a)\right\|_B \\ &\times \|u(a+t\delta a)\|_V + \beta \left\|\sigma'(a;\delta a)\right\|_B \|u(a+t\delta a) - u(a)\|_V .\end{aligned}$$

By taking the limit $t \downarrow 0$, the right-hand side tends to zero since u is continuous and σ is directionally differentiable, we get $\|\delta u_t - w\|_V \to 0$, which implies that $t^{-1}(u(a+t\delta a) - u(a)) \to w$ in V, and hence u is directionally differentiable at a in the direction δa with $u'(a;\delta a) = w$.

We follow similar arguments to prove the differentiability. For this we take a fixed a in the interior of A. Define the linear operator $T : B \to V$ such that for every $\delta a \in B$, $T(\delta a)$ gives the unique solution to the following variational equation:

$$T(\sigma(a), T(\delta a), v) = -T(D\sigma(a)(\delta a), u(a), v), \quad \text{for every } v \in V.$$

Since $-T(D\sigma(a)(\delta a), u(a), \cdot) \in V^*$, T is well defined. Furthermore,

$$\begin{aligned}\alpha \|T(\delta a)\|_V^2 &\le T(\sigma(a), T(\delta a), T(\delta a)) \\ &= -T(D\sigma(a)(\delta a), u(a), T(\delta a)) \\ &\le \beta \|D\sigma(a)(\delta a)\|_B \|T(\delta a)\|_V \|u(a)\|_V\end{aligned}$$

Since σ is differentiable we have $\|D\sigma(a)(\delta a)\|_B \le C \|\delta a\|_B$, and hence

$$\|T(\delta a)\|_V \le (\beta C \|u(a)\|_V) \|\delta a\|_B .$$

On the other hand, following the previous calculation, we have

$$T\left(\sigma(a), \frac{u(a+\delta a) - u(a)}{\|\delta a\|_B}, v\right) = -T\left(\frac{\sigma(a+\delta a) - \sigma(a)}{\|\delta a\|_B}, u(a+\delta a), v\right),$$

and therefore

$$\begin{aligned}T&\left(\sigma(a), \frac{u(a+\delta a) - u(a)}{\|\delta a\|_B}, v\right) - T\left(\sigma(a), T\left(\frac{\delta a}{\|\delta a\|_B}\right), v\right) \\ &= -T\left(\frac{\sigma(a+\delta a) - \sigma(a)}{\|\delta a\|_B}, u(a+\delta a), v\right) \\ &\quad + T\left(D\sigma(a)\left(\frac{\delta a}{\|\delta a\|_B}\right), u(a), v\right),\end{aligned}$$

or equivalently,

$$
\begin{aligned}
T&\left(\sigma(a), \frac{u(a+\delta a)-u(a)-T(\delta a)}{\|\delta a\|_B}, v\right) \\
&\qquad = -T\left(D\sigma(a)\left(\frac{\delta a}{\|\delta a\|_B}\right), u(a+\delta a)-u(a), v\right) \\
&\qquad - T\left(\frac{\sigma(a+\delta a)-\sigma(a)-D\sigma(a)\,(\delta a)}{\|\delta a\|_B}, u(a+\delta a), v\right).
\end{aligned}
$$

If we denote $\Delta u = \|\delta a\|_B^{-1}\left(u(a+\delta a)-u(a)-T(\delta a)\right) \in V$, then by following the same reasoning as for the previous case, we have

$$
\begin{aligned}
\alpha\,\|\Delta u\|_V^2 &\leq T\left(\sigma(a), \Delta u, \Delta u\right) \\
&= -T\left(\frac{\sigma(a+\delta a)-\sigma(a)-D\sigma(a)\,(\delta a)}{\|\delta a\|_B}, u(a+\delta a), \Delta u\right) \\
&+ T\left(D\sigma(a)\left(\frac{\delta a}{\|\delta a\|_B}\right), u(a+\delta a)-u(a), \Delta u\right),
\end{aligned}
$$

implying

$$
\begin{aligned}
\alpha\,\|\Delta u\|_V^2 \leq \Bigg(&\beta\frac{\|\sigma(a+\delta a)-\sigma(a)-D\sigma(a)\,(\delta a)\|_B}{\|\delta a\|_B}\,\|u(a+\delta a)\|_V \\
&+\beta\left\|D\sigma(a)\left(\frac{\delta a}{\|\delta a\|_B}\right)\right\|_B \|u(a+\delta a)-u(a)\|_V\Bigg)\,\|\Delta u\|_V
\end{aligned}
$$

and hence

$$
\begin{aligned}
\alpha\,\|\Delta u\|_V \leq\, &\beta\frac{\|\sigma(a+\delta a)-\sigma(a)-D\sigma(a)\,(\delta a)\|_B}{\|\delta a\|_B}\,\|u(a+\delta a)\|_V \\
&+ \beta\left\|D\sigma(a)\left(\frac{\delta a}{\|\delta a\|_B}\right)\right\|_B \|u(a+\delta a)-u(a)\|_V\,.
\end{aligned}
$$

Since u is continuous by hypothesis and σ is differentiable, we have

$$
\begin{aligned}
&\frac{\|\sigma(a+\delta a)-\sigma(a)-D\sigma(a)\,(\delta a)\|_B}{\|\delta a\|_B}\,\|u(a+\delta a)\|_V \\
&\qquad\qquad + \left\|D\sigma(a)\left(\frac{\delta a}{\|\delta a\|_B}\right)\right\|_B \|u(a+\delta a)-u(a)\|_V \to 0,
\end{aligned}
$$

for $\|\delta a\|_B \to 0$. Finally, for $\|\delta a\|_B \to 0$ and for any $v \in V$, we have

$$
\|\Delta u\|_V = \frac{\|u(a+\delta a)-u(a)-T(\delta a)\|_V}{\|\delta a\|_B} \to 0,
$$

and this ensures differentiability. The proof is complete. □

We have the following derivative formulas for the MOLS:

Theorem 2.4. *The MOLS functional* (2.2) *is directionally differentiable at any a in the interior of A. The first-order derivative is given by*

$$
J'(a;\delta a) = -\frac{1}{2}T\left(\sigma'(a;\delta a), u(a)+z, u(a)-z\right), \ \textit{for every}\ \ \delta a \in B. \tag{2.8}
$$

Proof. We fix an element a in the interior of A and let $\delta a \in B$ be also fixed. Set

$$\Delta J = 2\frac{J(a+t\delta a) - J(a)}{t}.$$

Then,

$$\begin{aligned}
\frac{\Delta J}{2} &= \frac{1}{t}\left[T(\sigma(a+t\delta a), u(a+t\delta a)-z, u(a+t\delta a)-z)\right.\\
&\left.-T(\sigma(a), u(a)-z, u(a)-z)\right]\\
&= \frac{1}{t}\left[T(\sigma(a+t\delta a), u(a+t\delta a)-z, u(a+t\delta a)-z)\right.\\
&\left.-T(\sigma(a), u(a+t\delta a)-z, u(a+t\delta a)-z)\right]\\
&+ \frac{1}{t}\left[T(\sigma(a), u(a+t\delta a)-z, u(a+t\delta a)-z) - T(\sigma(a), u(a)-z, u(a)-z)\right]\\
&= T\left(\frac{\sigma(a+t\delta a)-\sigma(a)}{t}, u(a+t\delta a)-z, u(a+t\delta a)-z\right)\\
&+ \frac{1}{t}\left[T(\sigma(a), u(a+t\delta a)-z, u(a+t\delta a)-z) - T(\sigma(a), u(a)-z, u(a)-z)\right]\\
&= T\left(\frac{\sigma(a+t\delta a)-\sigma(a)}{t}, u(a+t\delta a)-z, u(a+t\delta a)-z\right)\\
&+ \frac{1}{t}\left[T(\sigma(a), u(a+t\delta a)-z, u(a+t\delta a)-z)\right.\\
&\left.-T(\sigma(a), u(a)-z, u(a+t\delta a)-z)\right]\\
&+ \frac{1}{t}\left[T(\sigma(a), u(a)-z, u(a+t\delta a)-z) - T(\sigma(a), u(a)-z, u(a)-z)\right],
\end{aligned}$$

which further simplifies to

$$\begin{aligned}
\frac{\Delta J}{2} &= T\left(\frac{\sigma(a+t\delta a)-\sigma(a)}{t}, u(a+t\delta a)-z, u(a+t\delta a)-z\right)\\
&+ T\left(\sigma(a), \frac{u(a+t\delta a)-u(a)}{t}, u(a+t\delta a)-z\right)\\
&+ T\left(\sigma(a), u(a+t\delta a)-z, \frac{u(a+t\delta a)-u(a)}{t}\right)\\
&= T\left(\frac{\sigma(a+t\delta a)-\sigma(a)}{t}, u(a+t\delta a)-z, u(a+t\delta a)-z\right)\\
&+ 2T\left(\sigma(a), u(a+t\delta a)-z, \frac{u(a+t\delta a)-u(a)}{t}\right)\\
&= A_1(t) + A_2(t),
\end{aligned}$$

where

$$A_1(t) = T\left(\frac{\sigma(a+t\delta a)-\sigma(a)}{t}, u(a+t\delta a)-z, u(a+t\delta a)-z\right),$$
$$A_2(t) = 2T\left(\sigma(a), \frac{u(a+t\delta a)-u(a)}{t}, u(a+t\delta a)-z\right).$$

By using the following identities

$$\lim_{t\to 0} A_1(t) = T\left(\sigma'(a;\delta a), u(a)-z, u(a)-z\right)$$
$$\lim_{t\to 0} A_2(t) = 2T\left(\sigma(a), u'(a;\delta a), u(a)-z\right),$$

we obtain

$$\begin{aligned} J'(a,\delta a) &= \frac{1}{2}\lim_{t\to 0}\Delta J = \frac{1}{2}\lim_{t\to 0}\left[A_1(t)+A_2(t)\right] \\ &= \frac{1}{2}T\left(\sigma'(a;\delta a), u(a)-z, u(a)-z\right) + T\left(\sigma(a), u'(a;\delta a), u(a)-z\right) \\ &= \frac{1}{2}T\left(\sigma'(a;\delta a), u(a)-z, u(a)-z\right) - T(\sigma'(a;\delta a), u(a), u(a)-z) \\ [3pt] &= -\frac{1}{2}T\left(\sigma'(a;\delta a), u(a)+z, u(a)-z\right), \end{aligned}$$

where Theorem 2.3 was used. Since $\delta a \in B$ is arbitrary, we conclude that J is directionally differentiable. The proof is complete. $\square$

Remark 2.5. *The derivative characterization* (2.4) *is a natural extension of* (1.9) *and the derivative* (2.8) *is a natural extension of* (1.10).

We now proceed to give the second-order derivative for the MOLS:

Theorem 2.6. *The MOLS* (2.2) *is second-order directionally differentiable at anya in the interior of A. The second-order derivative, for any δa_1, $\delta a_2 \in X$, reads:*

$$\begin{aligned} J''(a;\delta a_1,\delta a_2) = &-\frac{1}{2}T\left(\sigma''(a;\delta a_1,\delta a_2), u(a)+z, u(a)-z\right) \\ &+ T(\sigma(a), u'(a,\delta a_1), u'(a,\delta a_2)) \end{aligned}$$

Proof. Setting

$$\Delta J = \frac{J'(a+t\delta a_2;\delta a_1) - J'(a;\delta a_1)}{t},$$

by Theorem 2.4, we have

$$\begin{aligned} \Delta J = &-\frac{1}{2t}\big[T\left(\sigma'(a+t\delta a_2;\delta a_1), u(a+t\delta a_2)+z, u(a+t\delta a_2)-z\right) \\ &- T\left(\sigma'(a;\delta a_1), u(a)+z, u(a)-z\right)\big] \end{aligned}$$

and

$$
\begin{aligned}
\Delta J = &-\frac{1}{2t}\big[T\left(\sigma'(a+t\delta a_2;\delta a_1), u(a+t\delta a_2)+z, u(a+t\delta a_2)-z\right)\\
&- T(\sigma'(a;\delta a_1), u(a+t\delta a_2)+z, u(a+t\delta a_2)-z)\big]\\
&- \frac{1}{2t}\big[T(\sigma'(a;\delta a_1), u(a+t\delta a_2)+z, u(a+t\delta a_2)-z)\\
&- T\left(\sigma'(a;\delta a_1), u(a)+z, u(a)-z\right)\big]\\
&= -\frac{1}{2}\left[T\left(t^{-1}\left(\sigma'(a+t\delta a_2;\delta a_1)-\sigma'(a;\delta a_1)\right)\right.\right.,\\
&u(a+t\delta a_2)+z, u(a+t\delta a_2)-z)]\\
&- \frac{1}{2t}\big[T(\sigma'(a;\delta a_1), u(a+t\delta a_2)-z, u(a+t\delta a_2)-z)\\
&- T\left(\sigma'(a;\delta a_1), u(a)+z, u(a+t\delta a_2)-z\right)\big]\\
&- \frac{1}{2t}\left[T(\sigma'(a;\delta a_1), u(a)+z, u(a+t\delta a_2)-z)\right.\\
&\left.-T\left(\sigma'(a;\delta a_1), u(a)+z, u(a)-z\right)\right]
\end{aligned}
$$

which becomes

$$
\begin{aligned}
\Delta J = &-\frac{1}{2}\left(T\left(t^{-1}\left(\sigma'(a+t\delta a_2;\delta a_1)-\sigma'(a;\delta a_1)\right)\right.\right.,\\
&u(a+t\delta a_2)+z, u(a+t\delta a_2)-z))\\
&-\frac{1}{2}T\left(\sigma'(a;\delta a_1), t^{-1}\left(u(a+t\delta a_2)-u(a)\right), u(a+t\delta a_2)-z\right)\\
&-\frac{1}{2}T\left(\sigma'(a;\delta a_1), u(a)+z, t^{-1}\left(u(a+t\delta a_2)-u(a)\right)\right)\\
&= -\frac{1}{2}B_1(t)-\frac{1}{2}B_2(t)-\frac{1}{2}B_3(t).
\end{aligned}
$$

where

$$
\begin{aligned}
B_1(t) &= T\left(t^{-1}\left(\sigma'(a+t\delta a_2;\delta a_1)-\sigma'(a;\delta a_1)\right)\right.,\\
&\qquad u(a+t\delta a_2)+z, u(a+t\delta a_2)-z)\\
B_2(t) &= T\left(\sigma'(a;\delta a_1), t^{-1}\left(u(a+t\delta a_2)-u(a)\right), u(a+t\delta a_2)-z\right)\\
B_3(t) &= T\left(\sigma'(a;\delta a_1), u(a)+z, t^{-1}\left(u(a+t\delta a_2)-u(a)\right)\right).
\end{aligned}
$$

Therefore,

$$\begin{aligned}
J''(a, \delta a_1, \delta a_2) &= \lim_{t\to 0}\left[-\frac{1}{2}B_1(t) - \frac{1}{2}B_2(t) - \frac{1}{2}B_3(t)\right] \\
&= -\frac{1}{2}T\left(\sigma''(a;\delta a_1, \delta a_2), u(a)+z, u(a)-z\right) \\
&\quad - \frac{1}{2}T(\sigma'(a;\delta a_1), u'(a;\delta a_2), u(a)-z) \\
&\quad - \frac{1}{2}T(\sigma'(a;\delta a_1), u(a)+z, u'(a;\delta a_2)) \\
&= -\frac{1}{2}T\left(\sigma''(a;\delta a_1, \delta a_2), u(a)+z, u(a)-z\right) \\
&\quad - T(\sigma'(a;\delta a_1), u'(a;\delta a_2), u(a)).
\end{aligned}$$

By applying Theorem 2.3, we obtain

$$\begin{aligned}
J''(a, \delta a_1, \delta a_2) &= -\frac{1}{2}T\left(\sigma''(a;\delta a_1, \delta a_2), u(a)+z, u(a)-z\right) \\
&\quad - T(\sigma'(a;\delta a_1), u'(a;\delta a_2), u(a)) \\
&= -\frac{1}{2}T\left(\sigma''(a;\delta a_1, \delta a_2), u(a)+z, u(a)-z\right) \\
&\quad + T(\sigma(a), u'(a;\delta a_1), u'(a;\delta a_2)),
\end{aligned}$$

and the proof is complete. □

Remark 2.7. *The second-order derivative is positive if*

$$\alpha\|u'(a,\delta a)\|_V^2 - \frac{1}{2}T\left(\sigma''(a;\delta a,\delta a), u(a)+z, u(a)-z\right) \geq 0,$$

uniformly. Clearly, if σ coincides with the identity map, then $\sigma'(a,\cdot) = id$, $\sigma''(a,\cdot,\cdot) = 0$ and we recover the formula corresponding to (1.11).

3. Finite dimensional approximation

In this section, we develop a discretization framework. Assume that we are given a parameter h converging to 0 and a family $\{V_h\}$ of finite dimensional subspaces of V. Analogously, we assume that B_h is a family of finite-dimensional subspaces of B. We set $A_h = B_h \cap A$ and assume that $\cap_{h=1}^{\infty} A_h \neq \emptyset$. Recall that H is compactly embedded in B and $A \subset H$. We assume that, for each $h > 0$, $P_h : V \to V_h$ and $\widetilde{P}_h : A \to A_h$ are the projection operators that satisfy

$$\|P_h v - v\|_V \to 0, \quad \text{for every } v \in V. \tag{3.1}$$

$$\|\widetilde{P}_h a - a\|_H \to 0, \quad \text{for every } a \in A. \tag{3.2}$$

The discrete analogue of (1.7) reads: Given $a_h \in A_h$, find $u_h \in V_h$ such that

$$T(\sigma(a_h), u_h, v_h) = m(v_h), \quad \text{for every } v_h \in V_h. \tag{3.3}$$

We consider the discrete minimization problem: Find $a_h^* \in A_h$ by solving

$$\min_{a_h \in A_h} J^h(a_h) = \frac{1}{2} T(\sigma(a_h), u_h - z, u_h - z) + \kappa \|a_h\|_H^2, \tag{3.4}$$

where u_h is the unique solution of (3.3).

The following result ensures the convergence of the discrete problem:

Theorem 3.1. *For each h, assume that $a_h^* \in A_h$ is a minimizer of* (3.4)*. Then there is a subsequence of $\{a_h^*\}$ that converges to a solution of the continuous optimization problem* (2.3)*.*

Proof. The solvability of (3.4) follows from the arguments used earlier. For all h, there exists a constant C such that $J^h(a_h^*) \leq C$, and hence $\{a_h^*\}$ is bounded in $\|\cdot\|_H$. Due to the compact embedding of H into B, there is a subsequence that converges strongly, in $\|\cdot\|_B$, to an element of A. We assume that $\{a_h^*\}$ converges, in $\|\cdot\|_B$, to some $a^* \in A$. Let u^* and u_h^* be the unique solutions of the corresponding variational problems for the parameters a^* and a_h^*, respectively. Note that the sequence $\{u_h^*\}$ is bounded, independently of h. Therefore, there exists a subsequence, still denoted by $\{u_h^*\}$, such that u_h^* converges weakly to some $u^* \in V$ as $h \to 0$. We claim that $u^* = u^*(a^*)$.

Let $v \in V$ be fixed. By taking $v_h = P_h v$, where P_h is given in (3.1), we get

$$\begin{aligned} m(v_h) &= T(\sigma(a_h^*), u_h^*, v_h) \\ &= T(\sigma(a^*), u_h^*, v) + T(\sigma(a_h^*), u_h^*, v_h - v) + T(\sigma(a_h^*) - \sigma(a^*), u_h^*, v). \end{aligned} \tag{3.5}$$

The weak convergence of $\{u_h^*\}$ to u^* gives $T(\sigma(a^*), u_h^*, v) \to T(\sigma(a^*), u^*, v)$. By using (3.1), we obtain $|T(\sigma(a_h^*), u_h, v_h - v)| \leq \beta \|u_h^*\|_V \|v_h - v\|_V \to 0$. Since $a_h^* \to a^*$ in B, we have $|T(\sigma(a_h^*) - \sigma(a^*), u_h^*, v)| \to 0$. Finally, the convergence $v_h = P_h v \to v$ as $h \to 0$, implies that $m(v_h) \to m(v)$. Consequently, from (3.5), we infer that $T(\sigma(a^*), u^*, v) = m(v)$, for every $v \in V$, and since the variational problem is uniquely solvable for every $a \in A$, we deduce that $u^* = u^*(a^*)$. Since $\{a_h^*\} \subset A_h$ converges to $a^* \in A$ as $h \to 0$ in B, we can show that $T(\sigma(a_h^*), u_h^* - z, u_h^* - z) \to T(\sigma(a^*), u^* - z, u^* - z)$. This observation yields

$$\begin{aligned} J_\kappa(a^*) &= \frac{1}{2} T(\sigma(a^*), u^*(\sigma(a^*)) - z, u^*(a^*) - z) + \kappa \|a^*\|_H^2 \\ &\leq \lim_{h \to 0} \left\{ \frac{1}{2} T(\sigma(a_h^*), u_h^*(a_h^*) - z, u_h^*(a_h^*) - z) \right\} + \liminf_{h \to 0} \kappa \|a_h^*\|_H^2 \\ &\leq \liminf_{h \to 0} \left\{ \frac{1}{2} T(\sigma(a_h^*), u_h^*(a_h^*) - z, u_h^*(a_h^*) - z) + \kappa \|a_h^*\|_H^2 \right\}. \end{aligned}$$

Let $a \in A$ be arbitrary, and let $a_h = \widetilde{P}_h a$, where $\widetilde{P}_h$ is given in (3.2). We have

$$\begin{aligned} J_\kappa(a^*) &\leq \liminf_{h \to 0} \left\{ \frac{1}{2} T(\sigma(a_h^*), u_h^* - z, u_h^* - z) + \kappa \|a_h^*\|_H^2 \right\} \\ &\leq \liminf_{h \to 0} \left\{ \frac{1}{2} T(a_h, u_h(a_h) - z, u_h(a_h) - z) + \kappa \|a_h\|_H^2 \right\} \\ &= \frac{1}{2} T(a, u(a) - z, u(a) - z) + \kappa \|a\|_H^2 = J_\kappa(a), \end{aligned}$$

and since $a \in A$ was chosen arbitrarily, we deduce that a^* solves (2.3). $\square$

4. Computational framework

We begin with a triangulation T_h on Ω, L_h is the space of all piecewise continuous polynomials of degree d_a relative to T_h and V_h is the space of all piecewise continuous polynomials of degree d_u relative to T_h. Let the basis for A_h and V_h be given by $\{\varphi_1, \varphi_2, \ldots, \varphi_m\}$, and $\{\psi_1, \psi_2, \ldots, \psi_k\}$, respectively. For any $a \in L_h$, we define $A \in \mathbb{R}^m$ by $A_i = a(x_i)$, for $i = 1, 2, \ldots, m$, where the nodal basis $\{\varphi_1, \varphi_2, \ldots, \varphi_m\}$ corresponds to the nodes $\{x_1, x_2, \ldots, x_m\}$. Conversely, each $A \in \mathbb{R}^m$ corresponds to $a \in A_h$ defined by $a = \sum_{i=1}^m A_i \varphi_i$. We take $\sigma(a_h) = \sum_{i=1}^m \sigma(A_i)\varphi_i$ and $\sigma'(a_h) = \sum_{i=1}^m \sigma'(A_i)\varphi_i$. Similarly, $u \in V_h$ will correspond to $U \in \mathbb{R}^k$, where $U_i = u(z_i)$, $i = 1, 2, \ldots, k$, and $u = \sum_{i=1}^k U_i \psi_i$, where $z_1, z_2, \ldots, z_k$ are the nodes of the mesh defining V_h.

We define $S : \mathbb{R}^m \to \mathbb{R}^k$ to be the finite element solution operator that assigns to each $a_h \in A_h$, the unique solution $u_h \in V_h$ of the discrete problem (3.3) Then $S(A) = U$, where U is given by $K(A)U = F$, where $K(A)_{i,j} = T(\sigma(a), \psi_j, \psi_i)$, for $i, j = 1, 2, \ldots, k$.

The discrete MOLS function $J : \mathbb{R}^m \to \mathbb{R}$ is given by

$$J(A) = \frac{1}{2}(V - Z) \cdot K(A)(V - Z),$$

where V is defined by $S(A) = V$ and z is the discrete data. The gradient and the Hessian formulas can be easily deduced from this discrete version.

5. Numerical results

We now present some numerical results that demonstrate the successful identification of parameters using the MOLS functional. Recall that our goal is to identify the parameter a in the equation

$$-\nabla \cdot (\sigma(a)\nabla u) = f \quad \text{in } \Omega.$$

We consider homogeneous Dirichlet boundary condition along the entire boundary. Consider the problem in a two-dimensional domain $\Omega = [0, 1] \times [0, 1]$, the position vector is thus $x = (x_1, x_2)$. We choose the (exact) parameter a and the load function f as

$$a(x) = 1.5 + 0.2x_2^2 + 0.1(\sin(20x_1) + 1)$$
$$f(x) = 4 + 0.02(x_2 - 0.5)^2.$$

The following options for the parameter map are investigated:

$$\sigma_1(a) = a, \qquad \sigma_2(a) = a^3, \qquad \sigma_3(a) = \frac{1}{a}.$$

The measured solution z in each case is produced by first solving the forward problem with the exact parameter a and then adding random noise. The noise added to the measured solution z is from a uniform random distribution on the range $[-\alpha, \alpha]$ with $\alpha = 10^{-5}$. The regularization parameter for these computations is taken as $\kappa = 4 \cdot 10^{-6}$.

Figures 1-3 show reconstructions of a parameter a for parameter maps σ_1 through σ_3 using MOLS functional. Comparisons of exact and identified parameters in top rows show that the parameter is identified well for both linear σ_1 map where the functional is convex and nonlinear (σ_2, σ_3) where it is not convex. While the exact parameter is the same always, the magnitude of the solution u (lower right images) are very different for each parameter map, so the effect of the added random noise (which is the same $\alpha = 10^{-5}$) is different in each case. The noise adds some noticeable corruption in the reconstruction due to its relatively large magnitude especially in the case of parameter map σ_2. For this parameter map, the magnitude of the solution u is really small and the effect of the noise in reconstruction is clearly seen in the top right image of Figure 2.

All numerical experiments are carried out by using finite element library deal.II [3]. The computational framework is tested extensively by a set of example problems and it is shown to be quite robust. The computational cost of solving the inverse problem is significantly higher in cases of nonlinear parameter maps σ_2 and σ_3 than the linear map σ_1. For the case of linear parameter map, certain performance optimizations are possible and this makes the overall identification process very efficient.

We have also compared the performance of the new MOLS with the OLS. In all our experiments; the new MOLS was significantly faster than the OLS. This benefit of the new MOLS, however, was expected as the gradient computation of the OLS requires the computation of the derivative of the parameter-to-solution map. The proposed MOLS does not have any such requirement.

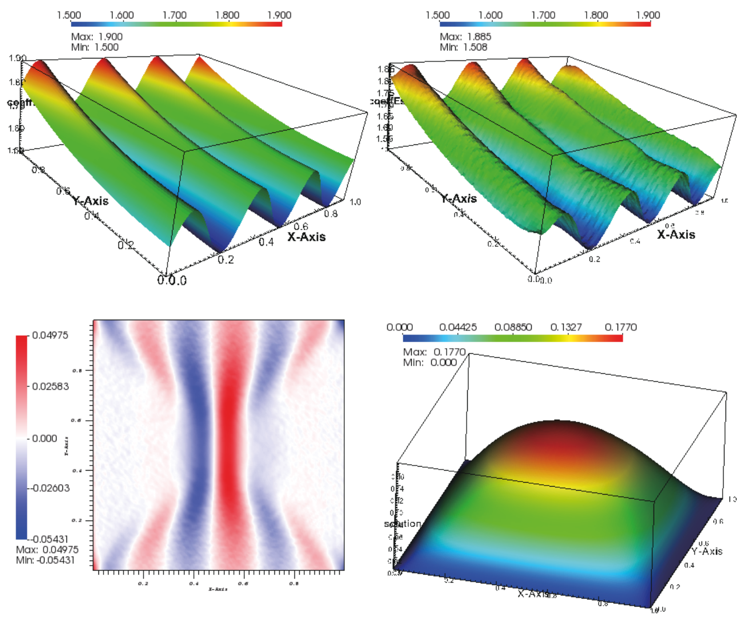

FIGURE 1. Exact and estimated parameters a and a_h (top row), error in parameter a (bottom left), and estimated solution u_h for the case of parameter map σ_1.

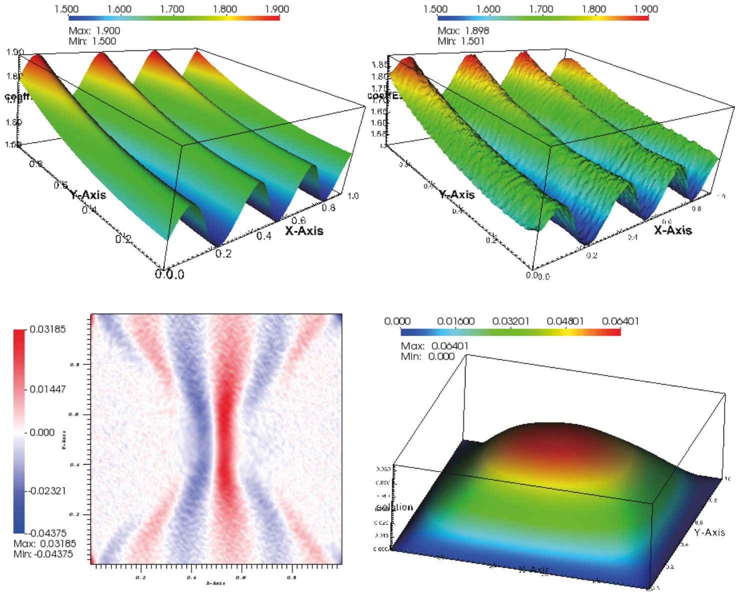

FIGURE 2. Exact and estimated parameters a and a_h (top row), error in parameter a (bottom left), and estimated solution u_h for the case of parameter map σ_2.

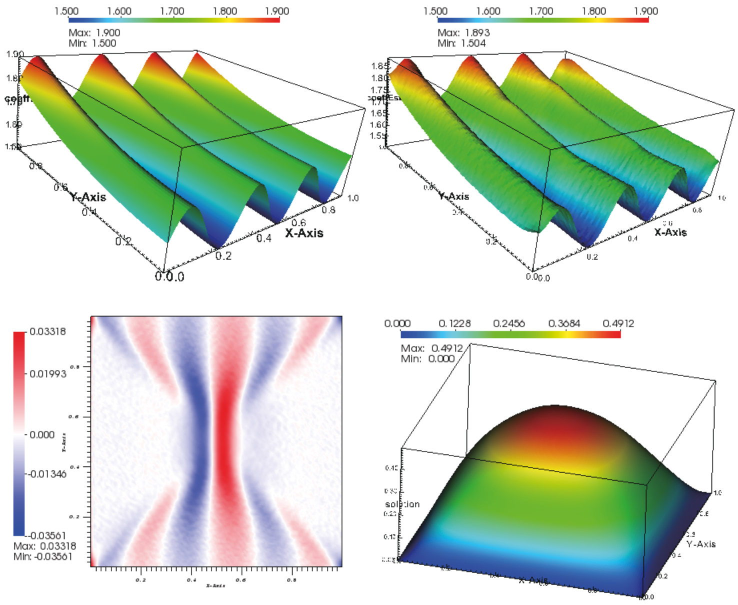

FIGURE 3. Exact and estimated parameters a and a_h (top row), error in parameter a (bottom left), and estimated solution u_h for the case of parameter map σ_3.

6. Concluding remarks

In this paper, we investigated the inverse problem of identifying parameters which appear nonlinearly in general variational problems. We proposed an extension of the MOLS and showed that the convexity of the original MOLS cannot be retained without additional assumptions. It would be of interest to further investigate the stability aspect of the considered inverse problem under data perturbation. The classical theory developed by Robinson [16] seems to pave the right path for such development.

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