Determination of thermal conductivity of inhomogeneous orthotropic materials from temperature measurements

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Abstract

We consider for the first time the two-dimensional inverse determination of the thermal conductivity of inhomogeneous orthotropic materials from internal temperature measurements. The inverse problem is general and is classified as a function estimation since no prior information about the functional form of the thermal conductivity is assumed in the inverse calculation. The least-squares functional minimizing naturally the gap between the measured and computed temperature leads to a set of direct, sensitivity and adjoint problems, which have forms of direct well-posed initial boundary value problems for the heat equation, and new formulas for its gradients are derived. The conjugate gradient method (CGM) employs recursively the solution of these problems at each iteration. Stopping the iterations according to the discrepancy principle criterion yields a stable solution. The employment of the Sobolev $W^{1,2}$-gradient is shown to result in much more robust and accurate numerical reconstructions than when the standard L^2-gradient is used.

Keywords: Heat equation; Thermal conductivity; Inverse problem; Conjugate gradient method; Orthotropic material

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1. Introduction

In the classical direct heat transfer problem, the cause (such as thermal conductivity) is given, and the effect (temperature field in the body) is determined. However, the inverse problem involves

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the estimation of the cause from the knowledge of the effect.

Difficulties encountered in the solution of the inverse problems should be recognized, since they are in general ill-posed. The solution of a well-posed problem needs to satisfy the requirements of existence, uniqueness and stability with respect to the input data. The existence of a solution for an inverse heat conduction problem may be assured according to physical reasoning. However, the uniqueness of the solution can be mathematically proved only for some special cases [1]. The solution of an inverse problem may become unstable, as a result of errors inherently present in measurements.

The use of inverse analysis for the estimation of thermal conductivity by utilizing steady [2] or transient temperature measurements taken within the medium and/or its boundary has numerous practical applications. The simultaneous determination of the thermal conductivity and heat capacity depending on space or temperature has been studied using the direct integration and Levenberg-Marquardt methods in [3, 4], respectively. The constant case of thermal conductivity has been identified in [5] and the temperature-dependent thermal conductivity was estimated by the Davidon-Fletcher-Powell method for the nonlinear inverse coefficient problem in [6]. In [7], a two-dimensional inverse coefficient problem has been studied to construct the time- and space-dependent thermal conductivity $k(x, y, t)$ of a non-homogeneous medium using the conjugate gradient method (CGM) from internal and boundary temperature measurements. The simultaneous determination of the space-dependent thermal conductivity and reaction coefficient has been considered in a one-dimensional inverse heat transfer problem using the CGM in [8]. Other applications of the CGM for the reconstruction of the heat transfer coefficient and the heat flux have recently been considered in [9, 10]. In this paper, we consider a two-dimensional coefficient identification problem to estimate the thermal conductivity of inhomogeneous orthotropic materials from internal temperature measurements. A quite different approach based on infrared thermography and pixels correlations has recently been proposed in [11].

Prior to this study, the identification of piecewise constant or linearly dependent functionally graded anisotropic materials was investigated in [12, 13, 14] using the genetic algorithm for the resulting finite dimensional optimization problem. However, in many materials, e.g. thermally bonded nonwovens, [15], the principal directions are orthogonal and then the anisotropic structure is called orthotropic. Such orthotropic structures have important characteristics and several inverse analyses have been unsertaken, [16, 17, 19, 18], for their estimation. Further, an experimental device for the simultaneous estimation of the constant thermal conductivity and the specific heat of orthotropic polymer composite materials was presented in [20]. However, in all these studies the material properties were piecewise constant or linearly space-dependent and this restricts the generality of the materials that can be identified. In reality, many materials are highly heterogeneous and therefore simplified assumptions such as having uniform or linearly varying in space properties are not appropriate. Therefore, in order to meet this generality manifested by inhomogeneous materials, in this paper we consider the more general infinite dimensional problem in which no prior information about the functional form of the thermal conductivity is assumed. Furthermore, the CGM is developed for solving iteratively the resulting optimization problem.

The CGM [1, 21, 22] derives from the perturbation principle and transforms the direct problem to the solution of two other related problems involved in the inverse analysis, namely, the sensitivity and the adjoint problems. In the following sections, we present the formulation of the direct problem which is used to obtain the temperature field $T(x, y, t)$. Then, we introduce the sensitivity and adjoint problems for the perturbation $\Delta T(x, y, t)$ and the Lagrange multiplier $\lambda(x, y, t)$, respectively. These three problems are repeatedly solved in the iterative CGM. For noisy data, the iterative process should be stopped according to the discrepancy principle or other similar stability criterion in order to prevent the instability setting in. The CGM is found to produce stable and accurate solutions for the thermal conductivity inside the spatial domain, but near the boundary the iterative algorithm does not evolve due to the gradient of the least-squares objective functional which is minimized vanishing at the boundary. In order to deal with this difficulty, the Sobolev gradient concept [1, 23, 24] is employed.

2. The direct problem

As a mathematical model, we consider a two-dimensional, transient heat transfer problem in an orthotropic square plate $\Omega = (0, 1) \times (0, 1)$, over the time interval from the initial time $t = 0$ to a given final time $t = t_f > 0$. The governing equation is given by the parabolic heat equation

$$\frac{\partial T}{\partial t}(x,y,t) = \frac{\partial}{\partial x}\left[k_{11}(x,y)\frac{\partial T}{\partial x}(x,y,t)\right] + \frac{\partial}{\partial y}\left[k_{22}(x,y)\frac{\partial T}{\partial y}(x,y,t)\right] - q(x,y)T(x,y,t)$$
$$+S(x,y,t), \quad (x,y,t) \in \Omega \times (0,t_f), \qquad (1)$$

where $T(x,y,t)$ is the temperature, $k_{11}(x,y) > 0$ and $k_{22}(x,y) > 0$ are the components of the orthotropic thermal conductivity tensor $\begin{bmatrix} k_{11} & 0 \\ 0 & k_{22} \end{bmatrix}$, $q(x,y) \geq 0$ is a known reaction coefficient, $S(x,y,t)$ is a known heat source and, for simplicity, the heat capacity has been assumed constant and taken to be unity.

We consider the Neumann heat flux boundary conditions

$$-k_{11}(0,y)\frac{\partial T}{\partial x}(0,y,t) = q_1(y,t), \quad k_{11}(1,y)\frac{\partial T}{\partial x}(1,y,t) = q_2(y,t), \quad (y,t) \in (0,1)\times(0,t_f), \qquad (2)$$
$$-k_{22}(x,0)\frac{\partial T}{\partial y}(x,0,t) = q_3(x,t), \quad k_{22}(x,1)\frac{\partial T}{\partial y}(x,1,t) = q_4(x,t), \quad (x,t) \in (0,1)\times(0,t_f), \qquad (3)$$

and the initial condition

$$T(x,y,0) = T_0(x,y), \quad (x,y) \in \overline{\Omega}, \qquad (4)$$

where $(q_i)_{i=\overline{1,4}}$ and T_0 are given functions. Dirichlet, mixed or Robin boundary conditions can also be considered.

The direct problem is concerned with the determination of the temperature $T(x,y,t)$ satisfying (1)–(4), when the thermal conductivity components $k_{11}(x,y)$ and $k_{22}(x,y)$ are known.

3. The inverse problem

The inverse problem, on the other hand, is concerned with the estimation of the unknown positive thermal conductivity components $k_{11}(x,y)$ and $k_{22}(x,y)$ by using the transient temperature readings taken by sensors at some appropriate locations (x_i, y_j), say $x_i = (i-1)/(I-1)$, $i = \overline{1,I}$, $y_j = (j-1)/(J-1)$ and $j = \overline{1,J}$. Let the temperature readings at these points over the period t_f be denoted by $Y(x_i, y_j, t) \equiv Y_{i,j}(t)$, $i = \overline{1,I}$, $j = \overline{1,J}$. These may be contaminated with noise. Note that the above locations are usually fixed and may not necessarily coincide with the finite-difference grid points that will be later on employed in the numerical implementation.

The solution of the inverse problem is sought by minimizing the following least-squares objective functional:

$$\begin{aligned} J[k_{11}, k_{22}] =& \frac{1}{2} \sum_{i=2}^{I-1} \sum_{j=2}^{J-1} \| T(x_i, y_j, t; k_{11}, k_{22}) - Y_{i,j}(t) \|^2_{L^2[0,t_f]} \\ =& \frac{1}{2} \int_0^{t_f} \sum_{i=2}^{I-1} \sum_{j=2}^{J-1} \left[T(x_i, y_j, t; k_{11}, k_{22}) - Y_{i,j}(t) \right]^2 dt. \end{aligned} \quad (5)$$

For simplicity, we consider in (5) only internal measurements of the temperature $Y_{i,j}(t)$ for $i = \overline{2, I-1}$, $j = \overline{2, J-1}$, noting that boundary temperature measurements can also be easily incorporated.

We note that previously Huang and Chin [7] considered the CGM for solving the problem of retrieving a both space- and time-dependent isotropic thermal conductivity $k(x, y, t)$ from temperature measurements $Y_{i,j}(t)$ for $i = \overline{1, I}$, $j = \overline{1, J}$.

4. The conjugate gradient method (CGM)

The CGM, [1, 22, 25], is an iterative method formed using three problems, namely: the direct problem mentioned in Section 2, the sensitivity problem, which will be described in Subsection 4.1 and the adjoint problem, which will be described in Subsection 4.2.

4.1. The sensitivity problem

The sensitivity problem is obtained from the original direct problem (1)–(4) with $k_{11}(x, y)$ and $k_{22}(x, y)$ known and $T(x, y, t)$ unknown. Let us suppose that the temperature $T(x, y, t)$ is perturbed by $\varepsilon \Delta T_{11}(x, y, t)$ when the thermal conductivity $k_{11}(x, y)$ undergoes the increment $\varepsilon \Delta k_{11}(x, y)$, where $\varepsilon > 0$ is a small number. Substracting the two corresponding direct problems, dividing with ε, and letting $\varepsilon \searrow 0$, we obtain the following sensitivity problem for $\Delta T_{11}(x, y, t)$:

$$\frac{\partial(\Delta T_{11})}{\partial t} = \frac{\partial}{\partial x} \left[k_{11} \frac{\partial(\Delta T_{11})}{\partial x} + \Delta k_{11} \frac{\partial T}{\partial x} \right] + \frac{\partial}{\partial y} \left[k_{22} \frac{\partial(\Delta T_{11})}{\partial y} \right] - q \Delta T_{11}, \quad (x, y, t) \in \Omega \times (0, t_f), \quad (6)$$

with the Neumann boundary conditions

$$-k_{11}(0,y)\frac{\partial(\Delta T_{11})}{\partial x}(0,y,t)=\Delta k_{11}(0,y)\frac{\partial T}{\partial x}(0,y,t),\quad (y,t)\in(0,1)\times(0,t_f), \tag{7}$$

$$k_{11}(1,y)\frac{\partial(\Delta T_{11})}{\partial x}(1,y,t)=-\Delta k_{11}(1,y)\frac{\partial T}{\partial x}(1,y,t),\quad (y,t)\in(0,1)\times(0,t_f), \tag{8}$$

$$-k_{22}(x,0)\frac{\partial(\Delta T_{11})}{\partial y}(x,0,t)=k_{22}(x,1)\frac{\partial(\Delta T_{11})}{\partial y}(x,1,t)=0,\quad (x,t)\in(0,1)\times(0,t_f), \tag{9}$$

and the initial condition

$$\Delta T_{11}(x,y,0)=0,\quad (x,y)\in\overline{\Omega}. \tag{10}$$

We stress that throughout the paper the symbol Δ does not denote the usual Laplacian operator.

The sensitivity problem established by the same approach for $\Delta T_{22}(x,y,t)$ is:

$$\frac{\partial(\Delta T_{22})}{\partial t}=\frac{\partial}{\partial x}\left[k_{11}\frac{\partial(\Delta T_{22})}{\partial x}\right]+\frac{\partial}{\partial y}\left[k_{22}\frac{\partial(\Delta T_{22})}{\partial y}+\Delta k_{22}\frac{\partial T}{\partial y}\right]-q\Delta T_{22},\quad (x,y,t)\in\Omega\times(0,t_f), \tag{11}$$

with the Neumann boundary conditions

$$-k_{11}(0,y)\frac{\partial(\Delta T_{22})}{\partial x}(0,y,t)=k_{11}(1,y)\frac{\partial(\Delta T_{22})}{\partial x}(1,y,t)=0,\quad (y,t)\in(0,1)\times(0,t_f), \tag{12}$$

$$-k_{22}(x,0)\frac{\partial(\Delta T_{22})}{\partial y}(x,0,t)=\Delta k_{22}(x,0)\frac{\partial T}{\partial y}(x,0,t),\quad (x,t)\in(0,1)\times(0,t_f), \tag{13}$$

$$k_{22}(x,1)\frac{\partial(\Delta T_{22})}{\partial y}(x,1,t)=-\Delta k_{22}(x,1)\frac{\partial T}{\partial y}(x,1,t),\quad (x,t)\in(0,1)\times(0,t_f), \tag{14}$$

and the initial condition

$$\Delta T_{22}(x,y,0)=0,\quad (x,y)\in\overline{\Omega}. \tag{15}$$

4.2. The adjoint problem

We can write the minimization of the functional $J[k_{11},k_{22}]$ as a constrained optimization problem, since the computed temperature $T(x_i,y_j,t;k_{11},k_{22})$ must satisfy the direct problem. In order to solve this constrained optimization problem, we can use the Lagrange multiplier method. Therefore, we consider the following extended objective functional:

$$J[k_{11},k_{22}] =\frac{1}{2}\int_0^{t_f}\sum_{i=2}^{I-1}\sum_{j=2}^{J-1}\left[T(x_i,y_j,t;k_{11},k_{22})-Y_{i,j}(t)\right]^2 dt$$
$$+\int_0^{t_f}\int_0^1\int_0^1 \lambda(x,y,t)\left\{\frac{\partial}{\partial x}\left[k_{11}\frac{\partial T}{\partial x}\right]+\frac{\partial}{\partial y}\left[k_{22}\frac{\partial T}{\partial y}\right]-qT+S-\frac{\partial T}{\partial t}\right\}dxdydt, \quad (16)$$

where $\lambda(x,y,t)$ is a Lagrange multiplier.

As in [22, 29], we can use the Dirac delta function δ to rewrite (16). Delta functions select in the continuous space (x,y) the point (x_i,y_j) that matches the temperature readings (assumed local here) and thus allow the double sum to be introduced under the integral operators. Then, we have

$$J[k_{11},k_{22}] =\int_0^{t_f}\int_0^1\int_0^1 \frac{1}{2}\sum_{i=2}^{I-1}\sum_{j=2}^{J-1}\left[T-Y\right]^2 \delta(x-x_i)\delta(y-y_j)dxdydt$$
$$+\int_0^{t_f}\int_0^1\int_0^1 \lambda(x,y,t)\left\{\frac{\partial}{\partial x}\left[k_{11}\frac{\partial T}{\partial x}\right]+\frac{\partial}{\partial y}\left[k_{22}\frac{\partial T}{\partial y}\right]-qT+S-\frac{\partial T}{\partial t}\right\}dxdydt, \quad (17)$$

where, for simplicity, we write T and Y instead of $T(x_i,y_j,t;k_{11},k_{22})$ and $Y_{i,j}(t)$, respectively, in the corresponding terms attached to the double sum. Alternatively, if one uses an infrared camera [11], the temperature reading (pixels) $Y_{i,j}(t)$ could be considered as the average temperature of the sample over a small square corresponding to the projection of the pixel. In that case, the Dirac delta functions could be replaced by rectangular window functions.

We can then define the directional derivatives of $J[k_{11},k_{22}]$ using (17) in the directions of the perturbation in $k_{11}(x,y)$ and $k_{22}(x,y)$ as

$$\Delta J_{11}=\lim_{\varepsilon\to 0}\frac{J[k_{11}+\varepsilon\Delta k_{11},k_{22}]-J[k_{11},k_{22}]}{\varepsilon}, \quad \Delta J_{22}=\lim_{\varepsilon\to 0}\frac{J[k_{11},k_{22}+\varepsilon\Delta k_{22}]-J[k_{11},k_{22}]}{\varepsilon}. \quad (18)$$

Now expanding the generic term $\left[T+\varepsilon\Delta T-Y\right]^2$ and neglecting the second-order terms of order ε^2, we obtain

$$\left[T+\varepsilon\Delta T-Y\right]^2\approx T^2+Y^2-2YT+2\varepsilon T\Delta T-2\varepsilon Y\Delta T=(T-Y)^2+2\varepsilon\Delta T(T-Y) \quad (19)$$

and then

$$
\begin{aligned}
&J[k_{11}+\varepsilon\Delta k_{11},k_{22}]\\
&=\int_0^{t_f}\int_0^1\int_0^1 \frac{1}{2}\sum_{i=2}^{I-1}\sum_{j=2}^{J-1}\left[(T-Y)^2+2\varepsilon\Delta T_{11}(T-Y)\right]\delta(x-x_i)\delta(y-y_j)dxdydt\\
&\quad+\int_0^{t_f}\int_0^1\int_0^1 \lambda\left\{\frac{\partial}{\partial x}\left[(k_{11}+\varepsilon\Delta k_{11})\frac{\partial(T+\varepsilon\Delta T_{11})}{\partial x}\right]+\frac{\partial}{\partial y}\left[k_{22}\frac{\partial(T+\varepsilon\Delta T_{11})}{\partial y}\right]\right.\\
&\quad\left.-q(T+\varepsilon\Delta T_{11})+S-\frac{\partial(T+\varepsilon\Delta T_{11})}{\partial t}\right\}dxdydt. \qquad (20)
\end{aligned}
$$

Now subtracting $J[k_{11},k_{22}]$ from $J[k_{11}+\varepsilon\Delta k_{11},k_{22}]$ and neglecting the second-order terms of order ε^2, we obtain

$$
\begin{aligned}
J[k_{11}+\varepsilon\Delta k_{11},k_{22}]-J[k_{11},k_{22}]&=\int_0^{t_f}\int_0^1\int_0^1\left\{\sum_{i=2}^{I-1}\sum_{j=2}^{J-1}\varepsilon\Delta T_{11}(T-Y)\delta(x-x_i)\delta(y-y_j)\right.\\
&\quad+\lambda\left\{\frac{\partial}{\partial x}\left[\varepsilon\Delta k_{11}\frac{\partial T}{\partial x}+k_{11}\frac{\partial(\varepsilon\Delta T_{11})}{\partial x}\right]+\frac{\partial}{\partial y}\left[k_{22}\frac{\partial(\varepsilon\Delta T_{11})}{\partial y}\right]\right.\\
&\quad\left.\left.-\varepsilon q\Delta T_{11}-\frac{\partial(\varepsilon\Delta T_{11})}{\partial t}\right\}\right\}dxdydt, \qquad (21)
\end{aligned}
$$

and using (18)

$$
\begin{aligned}
\Delta J_{11}&=\int_0^{t_f}\int_0^1\int_0^1\left\{\sum_{i=2}^{I-1}\sum_{j=2}^{J-1}\Delta T_{11}(T-Y)\delta(x-x_i)\delta(y-y_j)\right.\\
&\quad\left.+\lambda\left\{\frac{\partial}{\partial x}\left[\Delta k_{11}\frac{\partial T}{\partial x}+k_{11}\frac{\partial(\Delta T_{11})}{\partial x}\right]+\frac{\partial}{\partial y}\left[k_{22}\frac{\partial(\Delta T_{11})}{\partial y}\right]-q\Delta T_{11}-\frac{\partial(\Delta T_{11})}{\partial t}\right\}\right\}dxdydt. \qquad (22)
\end{aligned}
$$

Let us analyse each one of the integrals in the expressions of ΔJ_{11} using integration by parts, as follows:

$$
I_1=\int_0^{t_f}\int_0^1\int_0^1\frac{\partial(\Delta T_{11})}{\partial t}\lambda dxdydt=\int_0^1\int_0^1\left[\Delta T_{11}\lambda\Big|_{t=0}^{t_f}-\int_0^{t_f}\Delta T_{11}\frac{\partial\lambda}{\partial t}dt\right]dxdy, \qquad (23)
$$

$$
\begin{aligned}
I_2&=\int_0^{t_f}\int_0^1\int_0^1\frac{\partial}{\partial x}\left[k_{11}\frac{\partial(\Delta T_{11})}{\partial x}\right]\lambda dxdydt\\
&=\int_0^{t_f}\int_0^1\left[\left(k_{11}\frac{\partial(\Delta T_{11})}{\partial x}\lambda-k_{11}\Delta T_{11}\frac{\partial\lambda}{\partial x}\right)\Big|_{x=0}^{1}+\int_0^1\Delta T_{11}\frac{\partial}{\partial x}\left[k_{11}\frac{\partial\lambda}{\partial x}\right]dx\right]dydt, \qquad (24)
\end{aligned}
$$

$$I_3 = \int_0^{t_f}\int_0^1\int_0^1 \frac{\partial}{\partial x}\left[\Delta k_{11}\frac{\partial T}{\partial x}\right]\lambda dxdydt = \int_0^{t_f}\int_0^1 \left[\Delta k_{11}\frac{\partial T}{\partial x}\lambda\Big|_{x=0}^1 - \int_0^1 \Delta k_{11}\frac{\partial T}{\partial x}\frac{\partial \lambda}{\partial x}dx\right]dydt, \tag{25}$$

$$\begin{aligned} I_4 &= \int_0^{t_f}\int_0^1\int_0^1 \frac{\partial}{\partial y}\left[k_{22}\frac{\partial(\Delta T_{11})}{\partial y}\right]\lambda dxdydt \\ &= \int_0^{t_f}\int_0^1 \left[\left(k_{22}\frac{\partial(\Delta T_{11})}{\partial y}\lambda - k_{22}\Delta T_{11}\frac{\partial \lambda}{\partial y}\right)\Big|_{y=0}^1 + \int_0^1 \Delta T_{11}\frac{\partial}{\partial y}\left[k_{22}\frac{\partial \lambda}{\partial y}\right]dy\right]dxdt. \end{aligned} \tag{26}$$

Substituting these integrals into (22), we get

$$\begin{aligned} \Delta J_{11} = &\int_0^{t_f}\int_0^1\int_0^1 \Delta T_{11}\left\{\sum_{i=2}^{I-1}\sum_{j=2}^{J-1}(T-Y)\delta(x-x_i)\delta(y-y_j) + \frac{\partial \lambda}{\partial t}\right. \\ &\left.+\frac{\partial}{\partial x}\left[k_{11}\frac{\partial \lambda}{\partial x}\right] + \frac{\partial}{\partial y}\left[k_{22}\frac{\partial \lambda}{\partial y}\right] - q\lambda\right\}dxdydt - \int_0^{t_f}\int_0^1\int_0^1 \Delta k_{11}\frac{\partial T}{\partial x}\frac{\partial \lambda}{\partial x}dxdydt \\ &+\int_0^{t_f}\int_0^1 k_{22}\frac{\partial(\Delta T_{11})}{\partial y}\lambda\Big|_{y=0}^1 dxdt - \int_0^1\int_0^1 \Delta T_{11}\lambda|_{t=0}^{t_f}dydx - \int_0^{t_f}\int_0^1 k_{11}\Delta T_{11}\frac{\partial \lambda}{\partial x}\Big|_{x=0}^1 dydt \\ &-\int_0^{t_f}\int_0^1 k_{22}\Delta T_{11}\frac{\partial \lambda}{\partial y}\Big|_{y=0}^1 dxdt + \int_0^{t_f}\int_0^1 \left[k_{11}\frac{\partial(\Delta T_{11})}{\partial x} + \Delta k_{11}\frac{\partial T}{\partial x}\right]\lambda\Big|_{x=0}^1 dydt. \end{aligned} \tag{27}$$

By using (7)–(10) and (12)–(15) into (27), and to nullify the integrands containing ΔT_{11}, the Lagrange multiplier $\lambda(x,y,t)$ must be solution of the following adjoint problem:

$$\begin{aligned} \frac{\partial \lambda}{\partial t}(x,y,t) = &-\frac{\partial}{\partial x}\left[k_{11}(x,y)\frac{\partial \lambda}{\partial x}(x,y,t)\right] - \frac{\partial}{\partial y}\left[k_{22}(x,y)\frac{\partial \lambda}{\partial y}(x,y,t)\right] + q(x,y)\lambda(x,y,t) \\ &-\sum_{i=2}^{I-1}\sum_{j=2}^{J-1}(T(x,y,t;k_{11},k_{22}) - Y_{i,j}(t))\delta(x-x_i)\delta(y-y_j), \quad (x,y,t)\in\Omega\times(0,t_f), \end{aligned} \tag{28}$$

$$-k_{11}(0,y)\frac{\partial \lambda}{\partial x}(0,y,t) = k_{11}(1,y)\frac{\partial \lambda}{\partial x}(1,y,t) = 0, \quad (y,t)\in(0,1)\times(0,t_f), \tag{29}$$

$$-k_{22}(x,0)\frac{\partial \lambda}{\partial y}(x,0,t) = k_{22}(x,1)\frac{\partial \lambda}{\partial y}(x,1,t) = 0, \quad (x,t)\in(0,1)\times(0,t_f), \tag{30}$$

$$\lambda(x,y,t_f) = 0, \quad (x,y)\in\overline{\Omega}. \tag{31}$$

The adjoint problem can be transformed to an initial value problem by the change of variable $\bar{t} = t_f - t$. The following term remains in (27):

$$\Delta J_{11} = -\int_0^{t_f}\int_0^1\int_0^1 \Delta k_{11}(x,y)\frac{\partial T}{\partial x}\frac{\partial \lambda}{\partial x}dxdydt. \tag{32}$$

As the gradient functional J' of the functional J is defined by

$$\Delta J[k]_{L^2(\Omega)} = (J', \Delta k)_{L^2(\Omega)} = \int_0^1 \int_0^1 J'[k] \Delta k(x,y) dx dy, \tag{33}$$

we obtain that the gradient component

$$J'_{11}[k_{11}, k_{22}] = -\int_0^{t_f} \frac{\partial T}{\partial x}(x,y,t) \frac{\partial \lambda}{\partial x}(x,y,t) dt. \tag{34}$$

Similarly,

$$J'_{22}[k_{11}, k_{22}] = -\int_0^{t_f} \frac{\partial T}{\partial y}(x,y,t) \frac{\partial \lambda}{\partial y}(x,y,t) dt. \tag{35}$$

Equation (33) defines the L^2-gradient of the functional J. However, from (29), (30), (34) and (35) it can be seen that J' vanishes at the boundary $\partial\Omega$. Therefore, in the iterative process described later on in Subsection 4.4 the boundary values of the unknown thermal conductivity components k_{11} and k_{22} will stay fixed and equal to those of the initial guess. Thus, if the initial guess is not close to the exact solution on the boundary $\partial\Omega$, the numerical results will also be far from it. In order to deal with this difficulty, extra H^1-smoothness is imposed on the solution through the introduction of the Sobolev gradient, as described in the next subsection. Other ways to deal with J' vanishing on $\partial\Omega$ are suggested in [25] page 81.

4.3. The Sobolev gradient

We introduce the Sobolev gradient denoted by $J'_{W^{1,2}}$ for the unknown thermal conductivity components $k_{11}(x,y)$ and $k_{22}(x,y)$ assuming that they belong to the Sobolev functional space $W^{1,2}(\Omega) = H^1(\Omega) = \{u \in L^2(\Omega) | u_x \text{ and } u_y \in L^2(\Omega)\}$. This is obtained via the inner product in $W^{1,2}(\Omega)$ rather than the gradients (34) and (35) which were obtained in $L^2(\Omega)$. The Sobolev gradient is smoother than the L^2-gradient as it represents a regularization of the L^2-gradient in the Fourier space such that the oscillating modes are attenuated [23].

The Sobolev gradient $J'_{W^{1,2}}[k]$ is defined by, [1, 23, 24],

$$\Delta J[k]_{W^{1,2}(\Omega)} = (J'_{W^{1,2}}, \Delta k)_{W^{1,2}(\Omega)}, \tag{36}$$

where

$$(J'_{W^{1,2}}, \Delta k)_{W^{1,2}(\Omega)} = \int_0^1 \int_0^1 (r_0 \Delta k J'_{W^{1,2}} + r_1 \nabla(\Delta k) \cdot \nabla J'_{W^{1,2}})\, dxdy, \tag{37}$$

r_0 and r_1 are some given positive continuous weight functions, and k stands for k_{11} or k_{22}. Usually, we take $r_0 = 1$, [23], and vary r_1 giving the amount of regularization in the weighted inner product.

Using integration by parts, equation (36) can be transformed to the form without any partial derivatives of the increment $\Delta k(x, y)$ inside the integral, i.e.

$$\begin{aligned}
\Delta J[k]_{W^{1,2}(\Omega)} &= (J'_{W^{1,2}}, \Delta k)_{W^{1,2}(\Omega)} = \int_0^1 \int_0^1 (r_0 \Delta k J'_{W^{1,2}} + r_1 \nabla(\Delta k) \cdot \nabla (J'_{W^{1,2}}))\, dxdy \\
&= \int_0^1 \int_0^1 \left(r_0 \Delta k J'_{W^{1,2}} - \Delta k \frac{\partial}{\partial x}\left(r_1 \frac{\partial J'_{W^{1,2}}}{\partial x} \right) - \Delta k \frac{\partial}{\partial y}\left(r_1 \frac{\partial J'_{W^{1,2}}}{\partial y} \right) \right) dxdy \\
&\quad + \int_0^1 \Delta k r_1 \frac{\partial J'_{W^{1,2}}}{\partial x}\bigg|_{x=0}^{1} dy + \int_0^1 \Delta k r_1 \frac{\partial J'_{W^{1,2}}}{\partial y}\bigg|_{y=0}^{1} dx.
\end{aligned} \tag{38}$$

By setting $\frac{\partial J'_{W^{1,2}}}{\partial x}\Big|_{x=0}^{1} = \frac{\partial J'_{W^{1,2}}}{\partial y}\Big|_{y=0}^{1} = 0$ in (38), then we have

$$\Delta J[k]_{W^{1,2}(\Omega)} = \left(r_0 J'_{W^{1,2}} - \frac{\partial}{\partial x}\left(r_1 \frac{\partial J'_{W^{1,2}}}{\partial x} \right) - \frac{\partial}{\partial y}\left(r_1 \frac{\partial J'_{W^{1,2}}}{\partial y} \right), \Delta k \right)_{L_2(\Omega)}. \tag{39}$$

Thus we obtain the following problem for finding the Sobolev gradient $J'_{W^{1,2}}$:

$$r_0 J'_{W^{1,2}} - \frac{\partial}{\partial x}\left(r_1 \frac{\partial J'_{W^{1,2}}}{\partial x} \right) - \frac{\partial}{\partial y}\left(r_1 \frac{\partial J'_{W^{1,2}}}{\partial y} \right) = J', \quad (x, y) \in \Omega, \tag{40}$$

$$\frac{\partial J'_{W^{1,2}}}{\partial x}(0, y) = \frac{\partial J'_{W^{1,2}}}{\partial x}(1, y) = 0, \quad y \in [0, 1], \tag{41}$$

$$\frac{\partial J'_{W^{1,2}}}{\partial y}(x, 0) = \frac{\partial J'_{W^{1,2}}}{\partial y}(x, 1) = 0, \quad x \in [0, 1], \tag{42}$$

where J' is given by (34) or (35). Note that if k is known on the boundary $\partial\Omega$ then (41) and (42) are replaced by the homogeneous Dirichlet boundary conditions

$$J'_{W^{1,2}}(0, y) = J'_{W^{1,2}}(1, y) = 0, \quad y \in [0, 1], \tag{43}$$

$$J'_{W^{1,2}}(x, 0) = J'_{W^{1,2}}(x, 1) = 0, \quad x \in [0, 1]. \tag{44}$$

Standard finite differences, [26], are employed for solving the above Neumann or Dirichlet problem for the elliptic equation (40). To summarise, the Sobolev gradients for $k_{11}(x, y)$ and $k_{22}(x, y)$ can be calculated from (40)–(42) by replacing the J' in (40) by J'_{11} given by (34) and J'_{22}

given by (35), respectively.

4.4. Iteration

The following iterative process based on the CGM is now used for the simultaneous estimation of $k_{11}(x,y)$ and $k_{22}(x,y)$ by minimizing the objective functional (5):

$$k_{11}^{n+1}(x,y) = k_{11}^{n}(x,y) - \beta_{11}^{n} P_{11}^{n}(x,y), \quad n = 0,1,2,\cdots, \tag{45}$$

$$k_{22}^{n+1}(x,y) = k_{22}^{n}(x,y) - \beta_{22}^{n} P_{22}^{n}(x,y), \quad n = 0,1,2,\cdots, \tag{46}$$

where the superscript n denotes the number of iterations, $k_{11}^{0}(x,y)$ and $k_{22}^{0}(x,y)$ are the initial guesses, and β_{11}^{n} and β_{22}^{n} are the step search sizes in passing from iteration n to iteration $n+1$, and $P_{11}^{n}(x,y)$ and $P_{22}^{n}(x,y)$ are the directions of descent given by

$$P_{11}^{0}(x,y) = J_{11}'^{0}, \quad P_{11}^{n}(x,y) = J_{11}'^{n} + \gamma_{11}^{n} P_{11}^{n-1}(x,y), \quad n = 1,2,\cdots, \tag{47}$$

$$P_{22}^{0}(x,y) = J_{22}'^{0}, \quad P_{22}^{n}(x,y) = J_{22}'^{n} + \gamma_{22}^{n} P_{22}^{n-1}(x,y), \quad n = 1,2,\cdots. \tag{48}$$

Different expressions are available for the conjugate coefficients γ_{11}^{n} and γ_{22}^{n}. The Polak–Ribiere expression [1, 27] gives

$$\gamma_{11}^{n} = \frac{\int_0^1\int_0^1 J_{11}'^{n}\left\{J_{11}'^{n} - J_{11}'^{n-1}\right\}dxdy}{\int_0^1\int_0^1 \left\{J_{11}'^{n-1}\right\}^2 dxdy}, \quad n = 1,2,\ldots, \tag{49}$$

$$\gamma_{22}^{n} = \frac{\int_0^1\int_0^1 J_{22}'^{n}\left\{J_{22}'^{n} - J_{22}'^{n-1}\right\}dxdy}{\int_0^1\int_0^1 \left\{J_{22}'^{n-1}\right\}^2 dxdy}, \quad n = 1,2,\ldots, \tag{50}$$

while the Fletcher–Reeves [1, 27, 28] expression gives

$$\gamma_{11}^{n} = \frac{\int_0^1\int_0^1 \left\{J_{11}'^{n}\right\}^2 dxdy}{\int_0^1\int_0^1 \left\{J_{11}'^{n-1}\right\}^2 dxdy} \quad n = 1,2,\cdots, \tag{51}$$

$$\gamma_{22}^{n} = \frac{\int_0^1\int_0^1 \left\{J_{22}'^{n}\right\}^2 dxdy}{\int_0^1\int_0^1 \left\{J_{22}'^{n-1}\right\}^2 dxdy} \quad n = 1,2.\cdots. \tag{52}$$

Note that there is also another version of the conjugate coefficient introduced by Powell and Beale [29, 30]. Preliminary investigations showed that for the problem studied here there is not much difference between those versions and therefore, in order to make a choice, only the Fletcher–Reeves expressions (51) and (52) will be employed to illustrate the numerical results in Section 5.

To find suitable step search sizes β_{11}^n and β_{22}^n we proceed as follows. First, based on (5), (45) and (46), we have

$$J[k_{11}^{n+1}, k_{22}^{n+1}] = \frac{1}{2}\int_0^{t_f} \sum_{i=2}^{I-1}\sum_{j=2}^{J-1} \left[T(x_i, y_j, t; k_{11}^n - \beta_{11}^n P_{11}^n, k_{22}^n - \beta_{22}^n P_{22}^n) - Y_{i,j}(t)\right]^2 dt. \tag{53}$$

Then, we linearise the temperature $T(x_i, y_j, t; k_{11}^n - \beta_{11}^n P_{11}^n, k_{22}^n - \beta_{22}^n P_{22}^n)$ by the first-order Taylor series expansion (assuming that $\beta_{11}^n P_{11}^n$ and $\beta_{22}^n P_{22}^n$ are small)

$$\begin{aligned} T(x_i, y_j, t; k_{11}^n - \beta_{11}^n P_{11}^n, k_{22}^n - \beta_{22}^n P_{22}^n) &\approx T(x_i, y_j, t; k_{11}^n, k_{22}^n) - \beta_{11}^n P_{11}^n \frac{\partial T_{i,j}^n(t)}{\partial k_{11}^n} - \beta_{22}^n P_{22}^n \frac{\partial T_{i,j}^n(t)}{\partial k_{22}^n} \\ &\approx T(x_i, y_j, t; k_{11}^n, k_{22}^n) - \beta_{11}^n \Delta T_{11}^n - \beta_{22}^n \Delta T_{22}^n, \end{aligned} \tag{54}$$

where ΔT_{11}^n and ΔT_{22}^n are the solutions of the sensitivity problems (6)–(10) and (11)–(15) with $\Delta k_{11}^n = P_{11}^n$ and $\Delta k_{22}^n = P_{22}^n$. Then, introducing (54) into (53) we have

$$J[k_{11}^{n+1}, k_{22}^{n+1}] = \frac{1}{2}\int_0^{t_f} \sum_{i=2}^{I-1}\sum_{j=2}^{J-1} \left[T(x_i, y_j, t; k_{11}^n, k_{22}^n) - \beta_{11}^n \Delta T_{11}^n - \beta_{22}^n \Delta T_{22}^n - Y_{i,j}(t)\right]^2 dt. \tag{55}$$

To minimize (55) we calculate the partial derivatives of $J[k_{11}^{n+1}, k_{22}^{n+1}]$ with respect to β_{11}^n and β_{22}^n to obtain

$$\begin{aligned} \frac{\partial J}{\partial \beta_{11}^n} &= -\int_0^{t_f} \sum_{i=2}^{I-1}\sum_{j=2}^{J-1} \left[T(x_i, y_j, t; k_{11}^n, k_{22}^n) - \beta_{11}^n \Delta T_{11}^n - \beta_{22}^n \Delta T_{22}^n - Y_{i,j}(t)\right] \Delta T_{11}^n dt \\ &= -C_1 + \beta_{11}^n C_2 + \beta_{22}^n C_3, \end{aligned} \tag{56}$$

and

$$\begin{aligned} \frac{\partial J}{\partial \beta_{22}^n} &= -\int_0^{t_f} \sum_{i=2}^{I-1}\sum_{j=2}^{J-1} \left[T(x_i, y_j, t; k_{11}^n, k_{22}^n) - \beta_{11}^n \Delta T_{11}^n - \beta_{22}^n \Delta T_{22}^n - Y_{i,j}(t)\right] \Delta T_{22}^n dt \\ &= -C_4 + \beta_{11}^n C_3 + \beta_{22}^n C_5, \end{aligned} \tag{57}$$

where

$$C_1 = \int_0^{t_f} \sum_{i=2}^{I-1} \sum_{j=2}^{J-1} \left[T_{i,j}(t) - Y_{i,j}(t)\right] \Delta T_{11}^n dt,$$

$$C_2 = \int_0^{t_f} \sum_{i=2}^{I-1} \sum_{j=2}^{J-1} \left[\Delta T_{11}^n\right]^2 dt, \quad C_3 = \int_0^{t_f} \sum_{i=2}^{I-1} \sum_{j=2}^{J-1} \Delta T_{11}^n \Delta T_{22}^n dt,$$

$$C_4 = \int_0^{t_f} \sum_{i=2}^{I-1} \sum_{j=2}^{J-1} \left[T_{i,j}(t) - Y_{i,j}(t)\right] \Delta T_{22}^n dt, \quad C_5 = \int_0^{t_f} \sum_{i=2}^{I-1} \sum_{j=2}^{J-1} \left[\Delta T_{22}^n\right]^2 dt.$$

Finally, setting $\frac{\partial J}{\partial \beta_{11}^n} = \frac{\partial J}{\partial \beta_{22}^n} = 0$, we obtain the search step sizes β_{11}^n and β_{22}^n as follows:

$$\beta_{11}^n = \frac{C_1 C_5 - C_3 C_4}{C_2 C_5 - C_3^2}, \quad \beta_{22}^n = \frac{C_2 C_4 - C_1 C_3}{C_2 C_5 - C_3^2}. \tag{58}$$

Although from expression (58) it is not obvious that the step search sizes β_{11}^n and β_{22}^n are (for all n) sufficiently small for the first-order Taylor series expansion (54) to be valid, this was not encountered as an issue in the numerical experiments performed in the next section.

4.5. Stopping criterion

The iterative procedure given by equations (45) and (46) does not provide the CGM with the stabilization necessary for the minimization of the functional (5) to be classified as well-posed because of the errors inherently present in the measured temperature. However, the CGM may become well-posed if the discrepancy principle [1, 21, 22, 31, 32] is used to stop the iterative procedure. In this criterion, the iterative procedure is stopped at the iteration number n_s at which

$$J[k^{n_s}] \approx \frac{1}{2}\mu^2, \tag{59}$$

where

$$\mu = \sqrt{\int_0^{t_f} \sum_{i=2}^{I-1} \sum_{j=2}^{J-1} \left[Y_{i,j}(t) - Y_{i,j}^{exact}(t)\right]^2 dt}, \tag{60}$$

represents the amount of noise with which the temperature data $Y_{i,j}(t)$ may be contaminated, and Y^{exact} denotes the exact temperature data in the absence of noise generated from the analytical solution, if available, or from solving the direct problem numerically (with care not to commit an inverse crime).

4.6. Algorithm

The steps of the CGM algorithm for estimating the unknown thermal conductivities $k_{11}(x, y)$ and $k_{22}(x, y)$ are, as follows:

1 Choose initial guesses $k_{11}^0(x, y)$ and $k_{22}^0(x, y)$ and set $n = 0$.

2 Solve the direct problem (1)–(4) by applying alternating–direction–implicit (ADI) scheme, described in Appendix A, to compute $T(x, y, t; k_{11}^n, k_{22}^n)$ and $J[k_{11}^n, k_{22}^n]$ by equation (5).

3 Solve the adjoint problem (28)–(31) to compute the Lagrange multiplier $\lambda(x, y, t; k_{11}, k_{22})$, and the gradient $J'_{11}[k_{11}^n, k_{22}^n]$ and $J'_{22}[k_{11}^n, k_{22}^n]$ from the equations (34) and (35) (or the Sobolev gradient $J_{W^{1,2}}$, as described in Subsection 4.3). Compute the conjugate coefficients γ_{11}^n and γ_{22}^n, and the directions of descent $P_{11}^n(x, y)$ and $P_{11}^n(x, y)$.

4 Solve the sensitivity problems (6)–(10) and (11)–(15) to compute the sensitivity functions ΔT_{11} and ΔT_{22} by taking $\Delta k_{11}^n(x, y) = P_{11}^n(x, y)$ and $\Delta k_{22}^n(x, y) = P_{22}^n(x, y)$, and compute the search step sizes β_{11}^n and β_{22}^n by (58).

5 Compute $k_{11}^{n+1}(x, y)$ and $k_{22}^{n+1}(x, y)$ by (45) and (46).

6 The stopping condition is:

If $J[k_{11}^n, k_{22}^n] \approx \frac{1}{2}\mu^2$ go to step 7.

Else set $n = n + 1$ go to step 2.

7 End.

5. Numerical results and discussion

The finite-difference method (FDM), based on the ADI scheme described in Appendix A, is used to calculate $\Delta T(x, y, t; k_{11}, k_{22})$ and $\lambda(x, y, t; k_{11}, k_{22})$ in the sensitivity and adjoint problems, respectively. Note that in the adjoint problem, the source term contains the Dirac delta function which can be approximated by

$$\delta(x - x_i) \approx \frac{1}{a\sqrt{\pi}} e^{-(x-x_i)^2/a^2}, \quad i = \overline{1, I} \tag{61}$$

where a is a small positive constant taken as $a = 10^{-3}$. The trapezoidal rule is used to approximate all the integrals in this paper, e.g., for the objective functional (5), we have

$$\begin{aligned} J[k_{11}, k_{22}] =& \frac{1}{2} \sum_{i=2}^{I-1} \sum_{j=2}^{J-1} ||T(x_i, y_j, t; k_{11}, k_{22}) - Y_{i,j}(t)||^2_{L^2[0,t_f]} \\ \approx& \frac{\Delta t}{4} \sum_{i=2}^{I-1} \sum_{j=2}^{J-1} \left\{ (T^1_{i,j} - Y_{i,j}(t_1))^2 + 2 \sum_{l=2}^{L-1} (T^l_{i,j} - Y_{i,j}(t_l))^2 + (T^L_{i,j} - Y_{i,j}(t_L))^2 \right\}. \end{aligned} \quad (62)$$

Note that since $t_1 = 0$, due to the initial condition (4) we always have that the first term in the bracket of the right-hand side of (62) vanishes. Thus, (62) simplifies as

$$J[k_{11}, k_{22}] \approx \frac{\Delta t}{4} \sum_{i=2}^{I-1} \sum_{j=2}^{J-1} \left\{ 2 \sum_{l=2}^{L-1} (T^l_{i,j} - Y_{i,j}(t_l))^2 + (T^L_{i,j} - Y_{i,j}(t_L))^2 \right\}. \quad (63)$$

Next, we define the errors at the iteration number n by

$$E(k^n_{11}) = \sqrt{\frac{1}{IJ} \sum_{i=1}^{I} \sum_{j=1}^{J} ({k_{11}}^n_{i,j} - {k_{11}}^{exact}_{i,j})^2}, \quad (64)$$

$$E(k^n_{22}) = \sqrt{\frac{1}{IJ} \sum_{i=1}^{I} \sum_{j=1}^{J} ({k_{22}}^n_{i,j} - {k_{22}}^{exact}_{i,j})^2}. \quad (65)$$

The temperature measurements Y containing random errors are simulated by adding to Y^{exact} an error term generated from a normal distribution by MATLAB in the form:

$$Y = Y^{exact} + \text{random}('\text{Normal}', 0, \sigma, I, J, L). \quad (66)$$

where $\sigma = \frac{p}{100} \max_{(x,y) \in \overline{\Omega}, t \in [0,t_f]} |T(x, y, t)|$ is the standard deviation and $p\%$ represents the percentage of noise.

All the numerical results illustrated in the figures of this paper are obtained with the FDM mesh size $\Delta x = \Delta y = 0.05$, i.e. $I = J = 20$, and taking $t_f = 1$, the time step $\Delta t = 0.025$, i.e. $L = 40$, which were found sufficiently fine so as to ensure that any further decrease in it did not significantly affect the accuracy of the numerical results. Based on (63), it means that we have $(I - 2) \times (J - 2) \times (L - 1) = 18 \times 18 \times 39 = 12636$ temperature measurements to solve for $2 \times I \times J = 2 \times 20 \times 20 = 800$ thermal conductivity discrete unknowns, which is a highly over-determined situation. In the Sobolev gradient equation (40) we take $r_0 = 1$ and, by trial and error, $r_1 = 0.1$. Nevertheless, more rigorous choices of the parameters r_0 and r_1, dictating the amount of $W^{1,2}$ regularization, should be investigated in the future.

5.1. Example 1

We first consider an isotropic material with input data generated by

$$
\begin{aligned}
&q_1(y,t) = -\frac{1+y}{12}(1-e^{-t})(\pi\sin(\pi y)+\pi+1), \quad q_2(y,t) = \frac{2+y}{12}(1-e^{-t})(-\pi\sin(\pi y)+\pi+1),\\
&q_3(x,t) = -\frac{1+x}{12}(1-e^{-t})(\pi\sin(\pi x)+\pi+1), \quad q_4(x,t) = \frac{2+x}{12}(1-e^{-t})(-\pi\sin(\pi x)+\pi+1),\\
&q(x,y) = 0, \quad T_0(x,y) = 0,\\
&S(x,y,t) = \left(e^{-t} + \frac{\pi^2}{6}(1+x+y)(1-e^{-t})\right)\sin(\pi x)\sin(\pi y) + (\pi+1)e^{-t}(x+y)\\
&\qquad - \frac{1-e^{-t}}{12}(\pi\sin(\pi(x+y)) + 2\pi + 2), \qquad (67)\\
&T(x,y,t) = Y^{exact}(x,y,t) = (1-e^{-t})(\sin(\pi x_i)\sin(\pi y_j) + (\pi+1)(x_i+y_j)). \qquad (68)
\end{aligned}
$$

The analytical solution of the inverse problem is

$$k_{11}(x,y) = \frac{1+x+y}{12}, \quad k_{22}(x,y) = \frac{1+x+y}{12}. \qquad (69)$$

We can use the CGM algorithm described in Section 4 to reconstruct the unknown orthotropic coefficients k_{11} and k_{22}, or the CGM of [7] to identify just one unknown isotropic coefficient $k(x,y) = k_{11}(x,y) = k_{22}(x,y)$ given by (69). We take the initial guess

$$k^0(x,y) = k^0_{11}(x,y) = k^0_{22}(x,y) = \frac{1+x+y}{12} + \frac{1}{2}xy(1-x)(1-y), \qquad (70)$$

where k^0 is used for the CGM of [7], and k^0_{11}, k^2_{22} are used for the CGM of this work. The L^2-gradient is applied in both algorithms. From the numerical results with no noise $p = 0$ shown in Figure 1, it can be seen that the former method generates slightly more accurate results than the latter one, as expected, since the method in [7] considers the inverse problem with only one unknown isotropic coefficient k, whilst the current method is more general as it allows to simultaneously identify two unknown orthotropic coefficients k_{11} and k_{22}. We also mention that the initial guess (70) is within 20% of the true solution (69) which may be considered as not too far. For much farther initial guesses we report that the numerically obtained results were not so accurate and therefore they are not presented. Instead, as we shall see in the next example, the Sobolev $W^{1,2}$-gradient is able to overcome the dependence of a subjectively good initial guess.

5.2. Example 2

We now consider an orthotropic material with input data generated by

$$\begin{aligned}
&q_1(y,t) = -\frac{1+y}{12}e^{-t}(\pi\sin(\pi y)+\pi+1), \quad q_2(y,t) = \frac{2+y}{12}e^{-t}(-\pi\sin(\pi y)+\pi+1), \\
&q_3(x,t) = -\frac{1+0.5x}{12}e^{-t}(\pi\sin(\pi x)+\pi+1), \quad q_4(x,t) = \frac{2+0.5x}{12}e^{-t}(-\pi\sin(\pi x)+\pi+1), \\
&q(x,y) = 0, \quad T_0(x,y) = \sin(\pi x)\sin(\pi y) + (\pi+1)(x+y)+1, \\
&S(x,y,t) = -e^{-t}(\sin(\pi x)\sin(\pi y) + (\pi+1)(x+y)+1) - \frac{e^{-t}}{12}(2\pi+2+\pi\sin(\pi(x+y))) \\
&\qquad + \frac{\pi^2 e^{-t}}{12}(2+1.5x+2y)\sin(\pi x)\sin(\pi y), \qquad (71) \\
&Y(x,y,t) = Y^{exact}(x,y,t) = e^{-t}(\sin(\pi x_i)\sin(\pi y_j)+(\pi+1)(x_i+y_j)+1). \qquad (72)
\end{aligned}$$

The analytical solution of the inverse problem is

$$k_{11}(x,y) = \frac{1+x+y}{12}, \qquad (73)$$

$$k_{22}(x,y) = \frac{1+0.5x+y}{12}. \qquad (74)$$

In the first instance, we take the initial guesses for the thermal conductivity components $k_{11}(x,y)$ and $k_{22}(x,y)$ as

$$k_{11}^0(x,y) = \frac{1}{2}xy(1-x)(1-y) + \frac{1+x+y}{12}, \quad k_{22}^0(x,y) = \frac{1}{2}xy(1-x)(1-y) + \frac{1+0.5x+y}{12}, \qquad (75)$$

which ensure that the boundary values of the initial approximations are equal to the exact ones.

First, we present the results for exact data, i.e., $p = 0$, in (66). The numerical solutions of $k_{11}(x,y)$ and $k_{22}(x,y)$ are presented in Figures 2 and 3, respectively. Figure 2 shows that the numerical results are good approximations of the exact solution (73). Furthermore, the results obtained with the Sobolev $W^{1,2}$-gradient are more accurate than the ones obtained using the L^2-gradient. Similar conclusions can be derived from Figure 3. In addition, one can remark that the numerical solutions obtained with the standard L^2-gradient are not so smooth near the boundary, but the employment of the Sobolev $W^{1,2}$-gradient alleviates this problem and the improvement obtained is quite significant.

Figure 4 shows the minimization of the objective functional (5) and the errors (64) and (65), as functions of the number of iterations n. From this figure, the importance of the stopping criterion (59), which is necessary to prevent the noise amplification, can be observed. For the given amounts of noise $p \in \{2, 4, 6\}$ this yields very quick stopping iteration numbers of $n_s \in \{3, 2, 2\}$, respectively, for the L^2-gradient and $n_s \in \{4, 3, 2\}$, respectively, for the $W^{1,2}$-gradient, and those values are consistent with the error curves in Figures 4(b), (c), (e) and (f). One can observe that there is only a small decrease in the objective functional (5) from the initial to the final value due to the initial guesses (75) being quite close (within 20%) to the true values given by equations (73) and (74). However, we shall soon depart from this "good" initial guess when we will choose the rather arbitrary guess (76) below. Finally, Figures 5 and 6 show the numerical results for the thermal conductivity components $k_{11}(x, y)$ and $k_{22}(x, y)$ for $p \in \{2, 4, 6\}$ noise. From these figures it can be seen that the numerical results are significantly smoother, more accurate and stable when using the Sobolev $W^{1,2}$-gradient than when using the L^2-gradient.

Next, for an arbitrary initial guesses for the thermal conductivity components $k_{11}(x, y)$ and $k_{22}(x, y)$, say

$$k_{11}^0(x, y) = k_{22}^0(x, y) = \frac{1}{4}, \tag{76}$$

we apply the Sobolev $W^{1,2}$-gradient satisfying (40)–(42). With the initial guess (76), the stopping criterion (59) yields $n_s \in \{9, 6, 5\}$ for $p \in \{2, 4, 6\}$ noise, respectively. In case of no noise, i.e. $p = 0$, we stop the iterations at an arbitrary large threshold, say $n_s = 30$. Figures 7 and 8 show that the numerical solutions for the thermal conductivity components k_{11} and k_{22} are smooth, stable and they become more accurate as the amount of noise p decreases. Remark also that the standard L^2-gradient produced very inaccurate results for the initial guess (76) due to the incompatibility between (76) and (73), (74) on the boundary.

6. Conclusions

In this paper, the determination of two-dimensional space-dependent orthotropic thermal conductivity from internal temperature measurements has been accomplished using the CGM together with the discrepancy principle. The Sobolev gradient has been utilized in the CGM iterative algorithm to reconstruct smoother and significantly more accurate and stable numerical solutions. Regularization has been achieved by stopping the iterations at the level at which the least-squares objective functional, minimizing the gap between the computed and the measured temperature, becomes just below the noise threshold with which the data is contaminated. The numerical results illustrate that the CGM together with the discrepancy principle is an efficient stable regularization method. Furthermore, its robustness with respect to the independence on the initial guess has been further enhanced by using the Sobolev gradient concept. Further work will consider reconstruction of an inhomogeneous and fully anisotropic thermal conductivity.

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A.

In this appendix, we describe the ADI scheme employed for discretising the orthotropic heat equation (1). First, we construct a rectangular network of mesh size Δx, Δy over the unit square $\Omega = (0,1) \times (0,1)$ and consider the time step of size Δt, namely,

$$\begin{aligned} x_i &= (i-1)\Delta x, \quad i = \overline{1, I}, \quad \Delta x = 1/(I-1), \\ y_j &= (j-1)\Delta y, \quad j = \overline{1, J}, \quad \Delta y = 1/(J-1), \\ t_l &= (l-1)\Delta t, \quad l = \overline{1, L}, \quad \Delta t = t_f/(L-1). \end{aligned}$$

We approximate (1) as

$$\begin{aligned} \frac{T_{i,j}^{l+\frac{1}{2}} - T_{i,j}^{l}}{\frac{1}{2}\Delta t} &= \frac{k_{11i+\frac{1}{2},j}}{(\Delta x)^2} T_{i+1,j}^{l+\frac{1}{2}} - \frac{k_{11i+\frac{1}{2},j} + k_{11i-\frac{1}{2},j}}{(\Delta x)^2} T_{i,j}^{l+\frac{1}{2}} + \frac{k_{11i-\frac{1}{2},j}}{(\Delta x)^2} T_{i-1,j}^{l+\frac{1}{2}} \\ &+ \frac{k_{22i,j+\frac{1}{2}}}{(\Delta y)^2} T_{i,j+1}^{l} - \frac{k_{22i,j+\frac{1}{2}} + k_{22i,j-\frac{1}{2}}}{(\Delta y)^2} T_{i,j}^{l} + \frac{k_{22i,j-\frac{1}{2}}}{(\Delta y)^2} T_{i,j-1}^{l} - q_{i,j} T_{i,j}^{l} + S_{i,j}^{l}, \end{aligned} \tag{A1}$$

and

$$\begin{aligned} \frac{T_{i,j}^{l+1} - T_{i,j}^{l+\frac{1}{2}}}{\frac{1}{2}\Delta t} &= \frac{k_{11i+\frac{1}{2},j}}{(\Delta x)^2} T_{i+1,j}^{l+\frac{1}{2}} - \frac{k_{11i+\frac{1}{2},j} + k_{11i-\frac{1}{2},j}}{(\Delta x)^2} T_{i,j}^{l+\frac{1}{2}} + \frac{k_{11i-\frac{1}{2},j}}{(\Delta x)^2} T_{i-1,j}^{l+\frac{1}{2}} \\ &+ \frac{k_{22i,j+\frac{1}{2}}}{(\Delta y)^2} T_{i,j+1}^{l+1} - \frac{k_{22i,j+\frac{1}{2}} + k_{22i,j-\frac{1}{2}}}{(\Delta y)^2} T_{i,j}^{l+1} + \frac{k_{22i,j-\frac{1}{2}}}{(\Delta y)^2} T_{i,j-1}^{l+1} - q_{i,j} T_{i,j}^{l+\frac{1}{2}} + S_{i,j}^{l+\frac{1}{2}}, \end{aligned} \tag{A2}$$

where $T_{i,j}^l = T(x_i, y_j, t_l)$, $k_{11i,j} = k_{11}(x_i, y_j)$, $k_{22i,j} = k_{22}(x_i, y_j)$, $q_{i,j} = q(x_i, y_j)$ and $S_{i,j}^l = S(x_i, y_j, t_l)$. Rearranging (A1) and (A2) we obtain the ADI method [33], which has the accuracy of $O(\Delta t^2 + \Delta x^2 + \Delta y^2)$, namely,

$$\begin{aligned} & -\alpha_{i-\frac{1}{2},j} T_{i-1,j}^{l+\frac{1}{2}} + (2 + \alpha_{i-\frac{1}{2},j} + \alpha_{i+\frac{1}{2},j}) T_{i,j}^{l+\frac{1}{2}} - \alpha_{i+\frac{1}{2},j} T_{i+1,j}^{l+\frac{1}{2}} \\ & \quad = \beta_{i,j-\frac{1}{2}} T_{i,j-1}^{l} + (2 - \beta_{i,j-\frac{1}{2}} - \beta_{i,j+\frac{1}{2}} - \Delta t q_{i,j}) T_{i,j}^{l} + \beta_{i,j+\frac{1}{2}} T_{i,j+1}^{l} + \Delta t S_{i,j}^{l}, \end{aligned} \tag{A3}$$

and

$$\begin{aligned} & -\beta_{i,j-\frac{1}{2}} T_{i,j-1}^{l+1} + (2 + \beta_{i,j-\frac{1}{2}} + \beta_{i,j+\frac{1}{2}}) T_{i,j}^{l+1} - \beta_{i,j+\frac{1}{2}} T_{i,j+1}^{l+1} \\ & \quad = \alpha_{i-\frac{1}{2},j} T_{i-1,j}^{l+\frac{1}{2}} + (2 - \alpha_{i-\frac{1}{2},j} - \alpha_{i+\frac{1}{2},j} - \Delta t q_{i,j}) T_{i,j}^{l+\frac{1}{2}} + \alpha_{i+\frac{1}{2},j} T_{i+1,j}^{l+\frac{1}{2}} + \Delta t S_{i,j}^{l+\frac{1}{2}}, \end{aligned} \tag{A4}$$

where $\alpha(x, y) = k_{11}(x, y)\Delta t/(\Delta x)^2$, $\beta(x, y) = k_{22}(x, y)\Delta t/(\Delta y)^2$, $\alpha_{i,j} = \alpha(x_i, y_j)$, $\beta_{i,j} = \beta(x_i, y_j)$, $\alpha_{i\pm 1/2,j} = (\alpha_{i,j} + \alpha_{i\pm 1,j})/2$ and $\beta_{i,j\pm 1/2} = (\beta_{i,j} + \beta_{i,j\pm 1})/2$.

Next, we discretise the Neumann boundary conditions (2)–(3) as

$$T_{1,j}^{l} = (4T_{2,j}^{l} - T_{3,j}^{l} + 2\Delta x (q_1)_j^l / k_{11\,1,j})/3, \quad T_{I,j}^{l} = (4T_{I-1,j}^{l} - T_{I-2,j}^{l} + 2\Delta x (q_2)_j^l / k_{11\,I,j})/3, \tag{A5}$$

$$T_{i,1}^{l} = (4T_{i,2}^{l} - T_{i,3}^{l} + 2\Delta y (q_3)_i^l / k_{22\,i,1})/3, \quad T_{i,J}^{l} = (4T_{i,J-1}^{l} - T_{i,J-2}^{l} + 2\Delta y (q_4)_i^l / k_{22\,i,J})/3. \tag{A6}$$

Introducing (A5) and (A6) into (A3) and (A4) we obtain

$$\boldsymbol{A}_j \boldsymbol{T}_j^{l+\frac{1}{2}} = \boldsymbol{f}_j^l, \quad j = \overline{2, J-1}, \tag{A7}$$

and

$$\boldsymbol{B}_i \boldsymbol{T}_i^{l+1} = \boldsymbol{f}_i^{l+\frac{1}{2}}, \quad i = \overline{2, I-1}, \tag{A8}$$

where

$$\boldsymbol{A}_j = \begin{bmatrix} 2 - \frac{1}{3}\alpha_{\frac{3}{2},j} + \alpha_{\frac{5}{2},j} & \frac{1}{3}\alpha_{\frac{3}{2},j} - \alpha_{\frac{5}{2},j} & & & \\ -\alpha_{\frac{5}{2},j} & 2 + \alpha_{\frac{5}{2},j} + \alpha_{\frac{7}{2},j} & -\alpha_{\frac{7}{2},j} & & \\ \ddots & \ddots & \ddots & & \\ & & -\alpha_{I-\frac{5}{2},j} & 2 + \alpha_{I-\frac{3}{2},j} + \alpha_{I-\frac{5}{2},j} & -\alpha_{I-\frac{3}{2},j} \\ & & & -\alpha_{I-\frac{3}{2},j} + \frac{1}{3}\alpha_{I-\frac{1}{2},j} & 2 + \alpha_{I-\frac{3}{2},j} - \frac{1}{3}\alpha_{I-\frac{1}{2},j} \end{bmatrix},$$

$$\boldsymbol{T}_j^{l+\frac{1}{2}} = \left[T_{2,j}^{l+\frac{1}{2}}, T_{3,j}^{l+\frac{1}{2}}, \cdots, T_{I-1,j}^{l+\frac{1}{2}} \right]^{\mathrm{T}},$$

$$
\boldsymbol{f}_j^l = \begin{bmatrix}
\beta_{2,j-\frac{1}{2}} T_{2,j-1}^l + (2 - \beta_{2,j-\frac{1}{2}} - \beta_{2,j+\frac{1}{2}} - \Delta t q_{2,j}) T_{2,j}^l + \beta_{2,j+\frac{1}{2}} T_{2,j+1}^l + \Delta t S_{2,j}^l \\
+\frac{2}{3} \Delta x \alpha_{\frac{3}{2},j} (q_1)_j^{l+\frac{1}{2}} / k_{111,j} \\
\beta_{3,j-\frac{1}{2}} T_{3,j-1}^l + (2 - \beta_{3,j-\frac{1}{2}} - \beta_{3,j+\frac{1}{2}} - \Delta t q_{3,j}) T_{3,j}^l + \beta_{3,j+\frac{1}{2}} T_{3,j+1}^l + \Delta t S_{3,j}^l \\
\vdots \\
\beta_{I-2,j-\frac{1}{2}} T_{I-2,j-1}^l + (2 - \beta_{I-2,j-\frac{1}{2}} - \beta_{I-2,j+\frac{1}{2}} - \Delta t q_{I-2,j}) T_{I-2,j}^l \\
+\beta_{I-2,j+\frac{1}{2}} T_{I-2,j+1}^l + \Delta t S_{I-2,j}^l \\
\beta_{I-1,j-\frac{1}{2}} T_{I-1,j-1}^l + (2 - \beta_{I-1,j-\frac{1}{2}} - \beta_{I-1,j+\frac{1}{2}} - \Delta t q_{I-1,j}) T_{I-1,j}^l \\
+\beta_{I-1,j+\frac{1}{2}} T_{I-1,j+1}^l + \Delta t S_{I-1,j}^l + \frac{2}{3} \Delta x \alpha_{I-\frac{1}{2},j} (q_2)_j^{l+\frac{1}{2}} / k_{11I,j}
\end{bmatrix},
$$

and

$$
\boldsymbol{B}_i = \begin{bmatrix}
2 - \frac{1}{3}\beta_{i,\frac{3}{2}} + \beta_{i,\frac{5}{2}} & \frac{1}{3}\beta_{i,\frac{3}{2}} - \beta_{i,\frac{5}{2}} & & & \\
-\beta_{i,\frac{5}{2}} & 2 + \beta_{i,\frac{5}{2}} + \beta_{i,\frac{7}{2}} & -\beta_{i,\frac{7}{2}} & & \\
\ddots & \ddots & \ddots & & \\
& -\beta_{i,J-\frac{5}{2}} & 2 + \beta_{i,J-\frac{3}{2}} + \beta_{i,J-\frac{5}{2}} & -\beta_{i,J-\frac{3}{2}} & \\
& & -\beta_{i,J-\frac{3}{2}} + \frac{1}{3}\beta_{i,J-\frac{1}{2}} & 2 + \beta_{i,J-\frac{3}{2}} - \frac{1}{3}\beta_{i,J-\frac{1}{2}} &
\end{bmatrix},
$$

$$
\boldsymbol{T}_i^{l+1} = \left[T_{i,2}^{l+1}, T_{i,3}^{l+1}, \cdots, T_{i,J-1}^{l+1} \right]^{\mathrm{T}},
$$

$$
\boldsymbol{f}_i^{l+\frac{1}{2}} = \begin{bmatrix}
\alpha_{i-\frac{1}{2},2} T_{i-1,2}^{l+\frac{1}{2}} + (2 - \alpha_{i-\frac{1}{2},2} - \alpha_{i+\frac{1}{2},2} - \Delta t q_{i,2}) T_{i,2}^{l+\frac{1}{2}} + \alpha_{i+\frac{1}{2},2} T_{i+1,2}^{l+\frac{1}{2}} + \Delta t S_{i,2}^{l+\frac{1}{2}} \\
+\frac{2}{3} \Delta y \beta_{i,\frac{3}{2}} (q_3)_i^{l+1} / k_{22i,1} \\
\alpha_{i-\frac{1}{2},3} T_{i-1,3}^{l+\frac{1}{2}} + (2 - \alpha_{i-\frac{1}{2},3} - \alpha_{i+\frac{1}{2},3} - \Delta t q_{i,3}) T_{i,3}^{l+\frac{1}{2}} + \alpha_{i+\frac{1}{2},3} T_{i+1,3}^{l+\frac{1}{2}} + \Delta t S_{i,3}^{l+\frac{1}{2}} \\
\vdots \\
\alpha_{i-\frac{1}{2},J-2} T_{i-1,J-2}^{l+\frac{1}{2}} + (2 - \alpha_{i-\frac{1}{2},J-2} - \alpha_{i+\frac{1}{2},J-2} - \Delta t q_{i,J-2}) T_{i,J-2}^{l+\frac{1}{2}} \\
+\alpha_{i+\frac{1}{2},J-2} T_{i+1,J-2}^{l+\frac{1}{2}} + \Delta t S_{i,J-2}^{l+\frac{1}{2}} \\
\alpha_{i-\frac{1}{2},J-1} T_{i-1,J-1}^{l+\frac{1}{2}} + (2 - \alpha_{i-\frac{1}{2},J-1} - \alpha_{i+\frac{1}{2},J-1} - \Delta t q_{i,J-1}) T_{i,J-1}^{l+\frac{1}{2}} \\
+\alpha_{i+\frac{1}{2},J-1} T_{i+1,J-1}^{l+\frac{1}{2}} + \Delta t S_{i,J-1}^{l+\frac{1}{2}} + \frac{2}{3} \Delta y \beta_{i,J-\frac{1}{2}} (q_4)_i^{l+1} / k_{22i,J}
\end{bmatrix}.
$$

NOMENCLATURE

E	root-mean-square error	t	time variable
J	objective functional	t_f	final time
J'	gradient of objective functional	x, y	space coordinates
$J'_{W^{1,2}}$	Sobolev gradient	Y	temperature data
$k_{11},\ k_{22}$	thermal conductivity components	Y^{exact}	exact temperature
n	number of iterations	β	search step size
P	direction of decent	γ	conjugate coefficient
q	perfusion coefficient	ε	small perturbation
q_1, q_2, q_3, q_4	heat fluxes	δ	Dirac delta function
r_0, r_1	weight functions	λ	Lagrange multiplier
S	source term	μ	amount of noise
T	temperature	σ	standard deviation
T_0	initial temperature		

List of Figures

$y = 0.6$ and (d) $y = 0.8$, for $p \in \{0, 2, 4, 6\}$ noise, for Example 2.

Figure 8 The exact (74) and numerical thermal conductivity component $k_{22}(x, y)$ obtained using the Sobolev $W^{1,2}$-gradient with the initial guess (76) at locations (a) $y = 0.2$, (b) $y = 0.4$, (c) $y = 0.6$ and (d) $y = 0.8$, for $p \in \{0, 2, 4, 6\}$ noise, for Example 2.

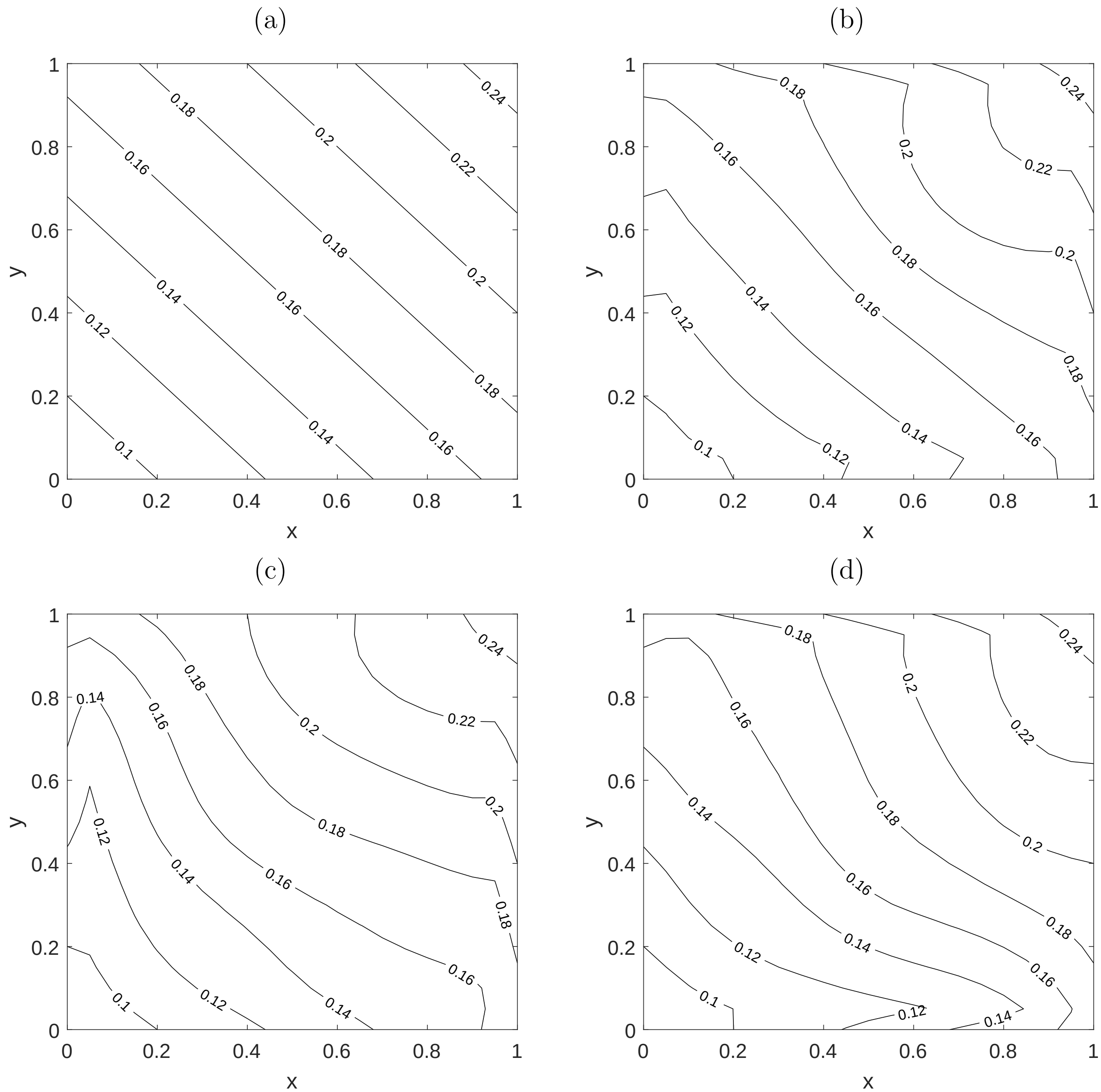

Figure 1: (a) The exact and numerical thermal conductivity (b) $k(x, y)$ obtained using the CGM of [7] for isotropic material in comparison with (c) $k_{11}(x, y)$ and (d) $k_{22}(x, y)$ obtained by the CGM of this paper for orthotropic material, for Example 1.

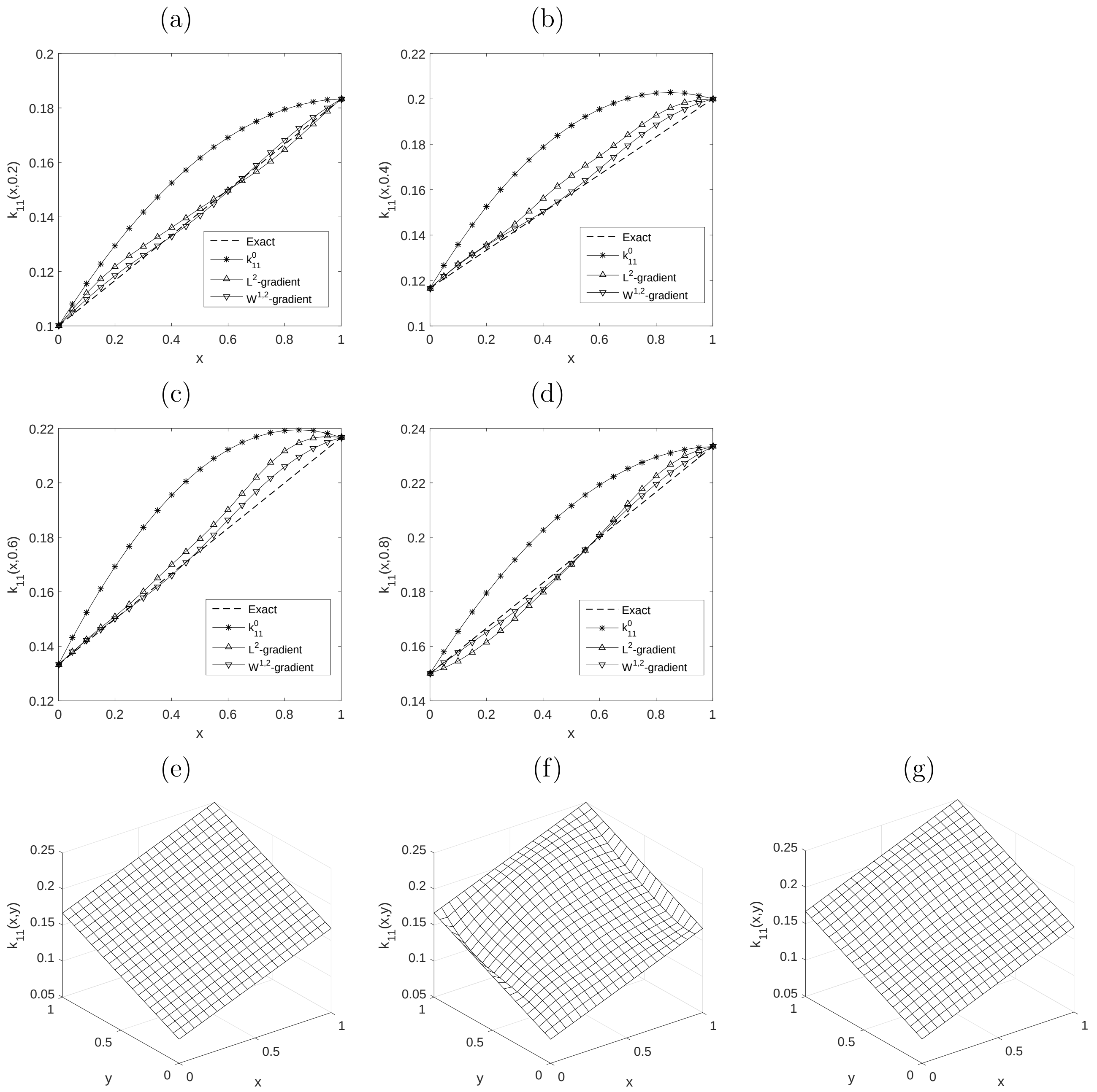

Figure 2: The exact (73) thermal conductivity component $k_{11}(x,y)$ together with the initial guess (75) and the numerical solutions at locations (a) $y = 0.2$, (b) $y = 0.4$, (c) $y = 0.6$ and (d) $y = 0.8$, for no noise, i.e., $p = 0$, obtained with the standard L^2-gradient and with the Sobolev $W^{1,2}$-gradient. (e) The exact $k_{11}(x,y)$, (f) $k_{11}(x,y)$ obtained by standard L^2-gradient and (g) $k_{11}(x,y)$ obtained by Sobolev $W^{1,2}$-gradient, for Example 2

.

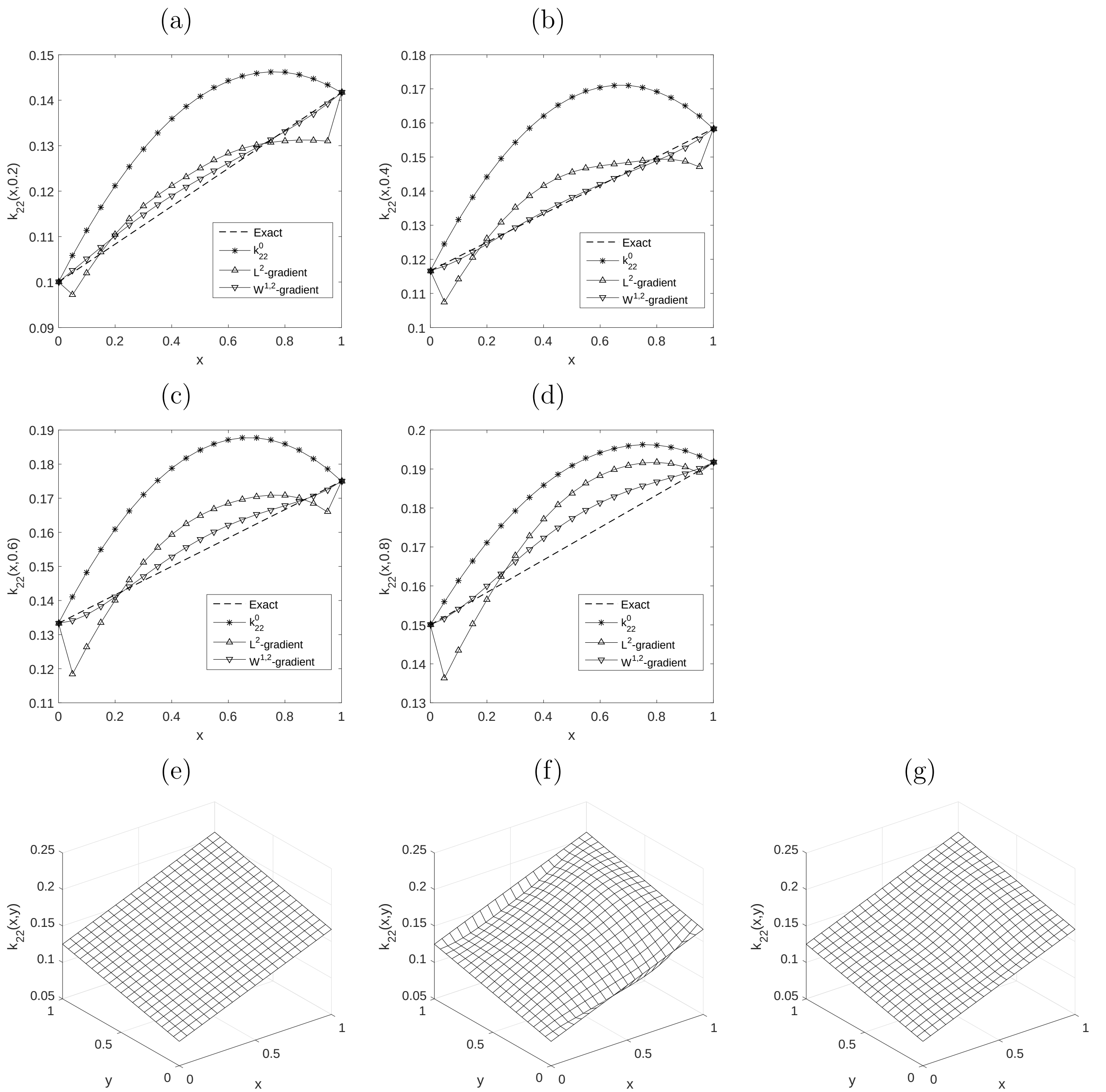

Figure 3: The exact (74) thermal conductivity component $k_{22}(x, y)$ together with the initial guess (75) and the numerical solutions at locations (a) $y = 0.2$, (b) $y = 0.4$, (c) $y = 0.6$ and (d) $y = 0.8$, for no noise, i.e., $p = 0$, obtained with the standard L^2-gradient and with the Sobolev $W^{1,2}$-gradient. (e) The exact $k_{22}(x, y)$, (f) $k_{22}(x, y)$ obtained by standard L^2-gradient and (g) $k_{22}(x, y)$ obtained by Sobolev $W^{1,2}$-gradient, for Example 2.

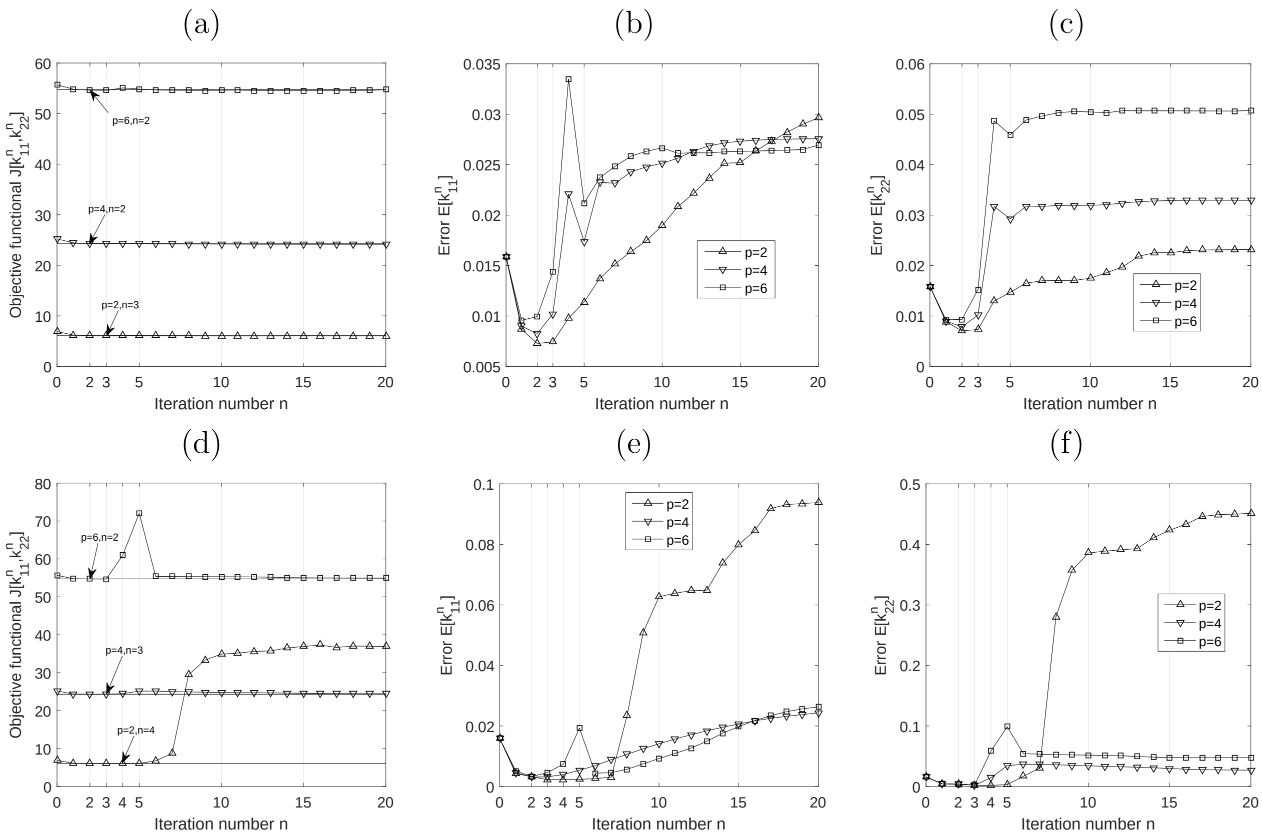

Figure 4: (a) The objective functional (5), (b) the error (64) and (c) the error (65), obtained with the initial guess (75) using the standard L^2-gradient (34) and (35), and the similar results (d)–(f) using the Sobolev $W^{1,2}$-gradient satisfying (40), (43) and (44), for $p \in \{2, 4, 6\}$ noise, for Example 2.

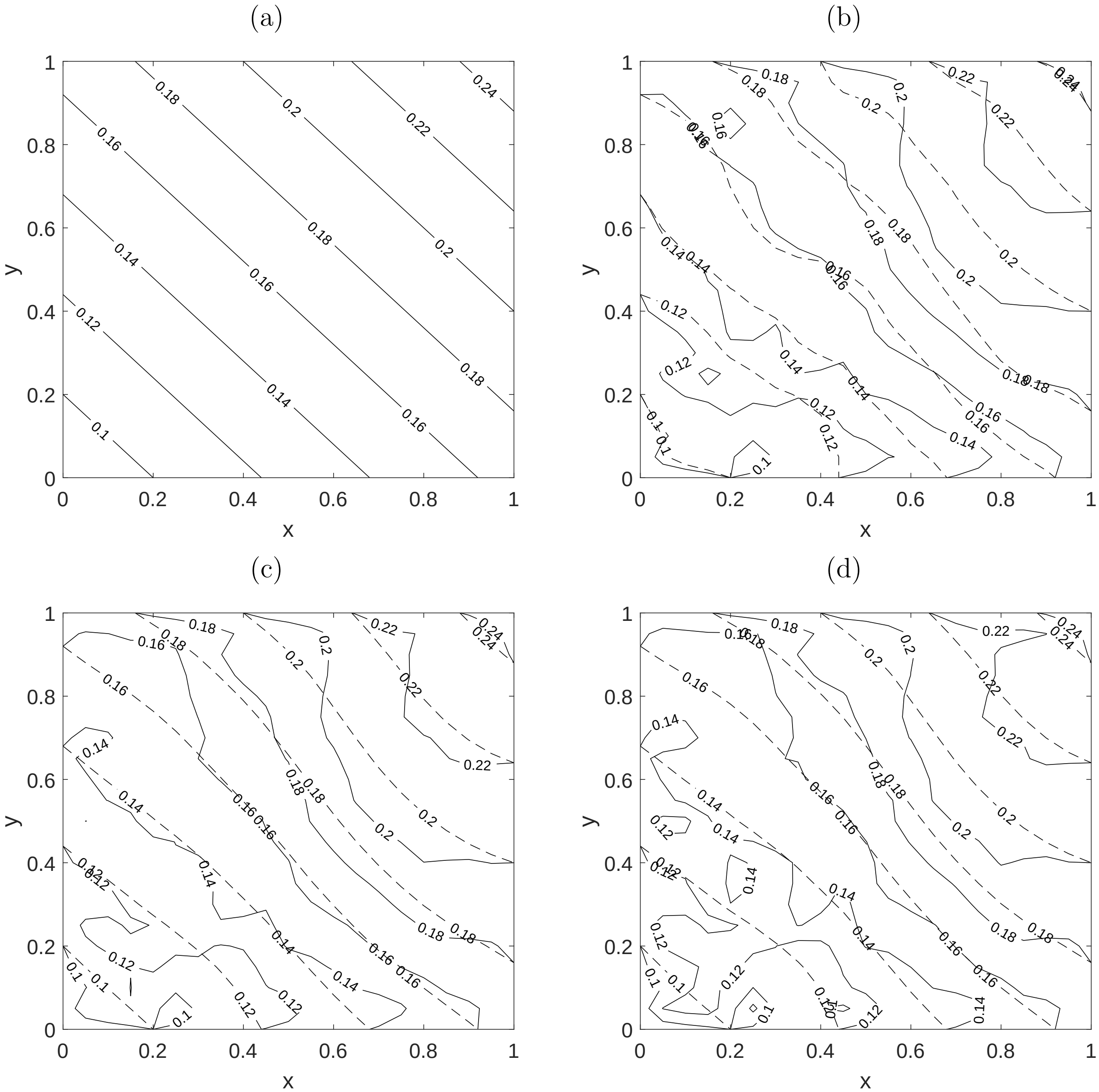

Figure 5: (a) The exact (73) and the numerical thermal conductivity component $k_{11}(x, y)$ obtained with the standard L^2-gradient (34) and (35) (——) and the Sobolev $W^{1,2}$-gradient (40), (43) and (44) (− − −) for (b) $p = 2$, (c) $p = 4$ and (d) $p = 6$ noise, for Example 2.

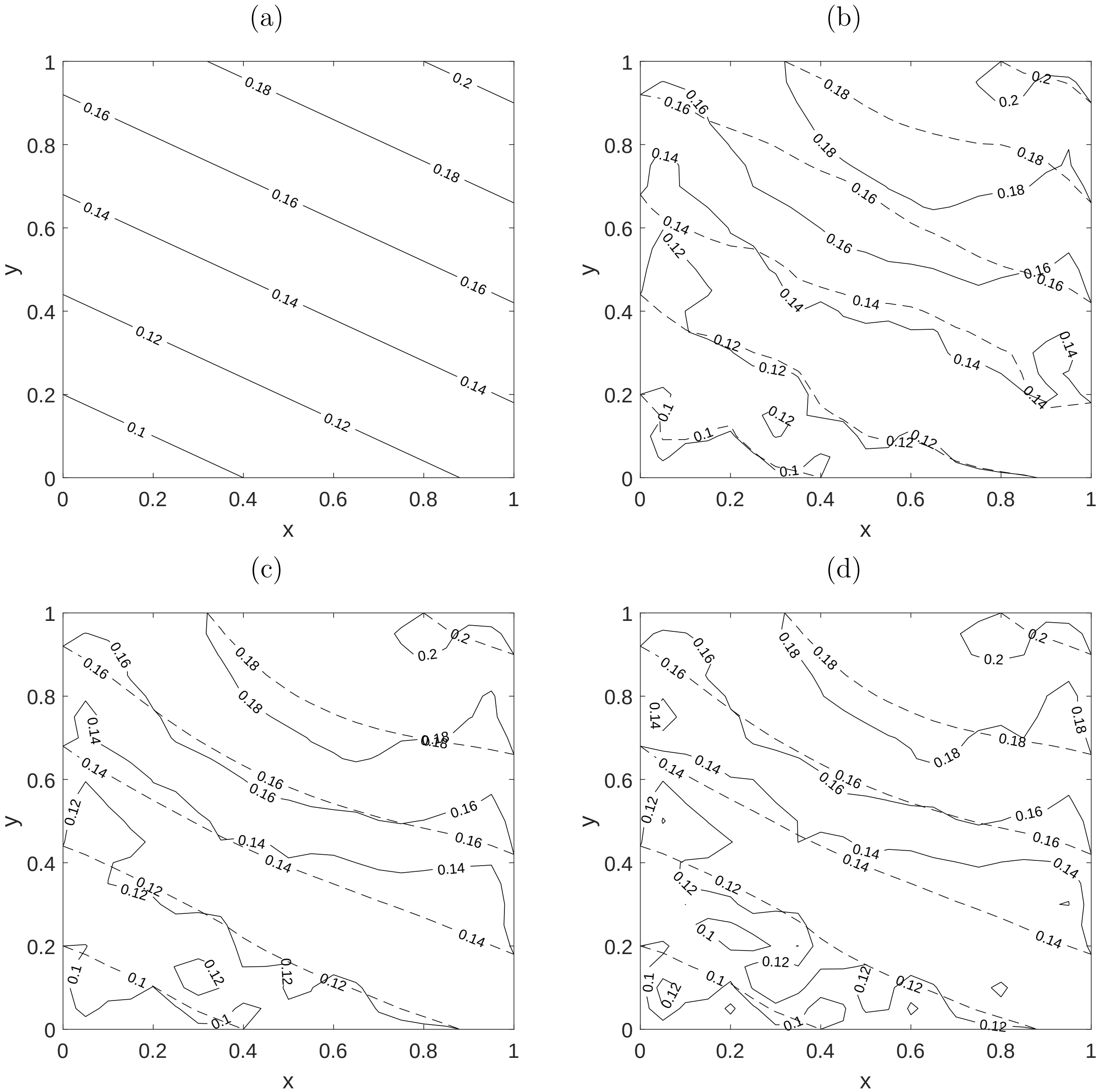

Figure 6: (a) The exact (74) and the numerical thermal conductivity component $k_{22}(x, y)$ obtained with the standard L^2-gradient (34) and (35) (——) and the Sobolev $W^{1,2}$-gradient (40), (43) and (44) (– – –) for (b) $p = 2$, (c) $p = 4$ and (d) $p = 6$ noise, for Example 2.

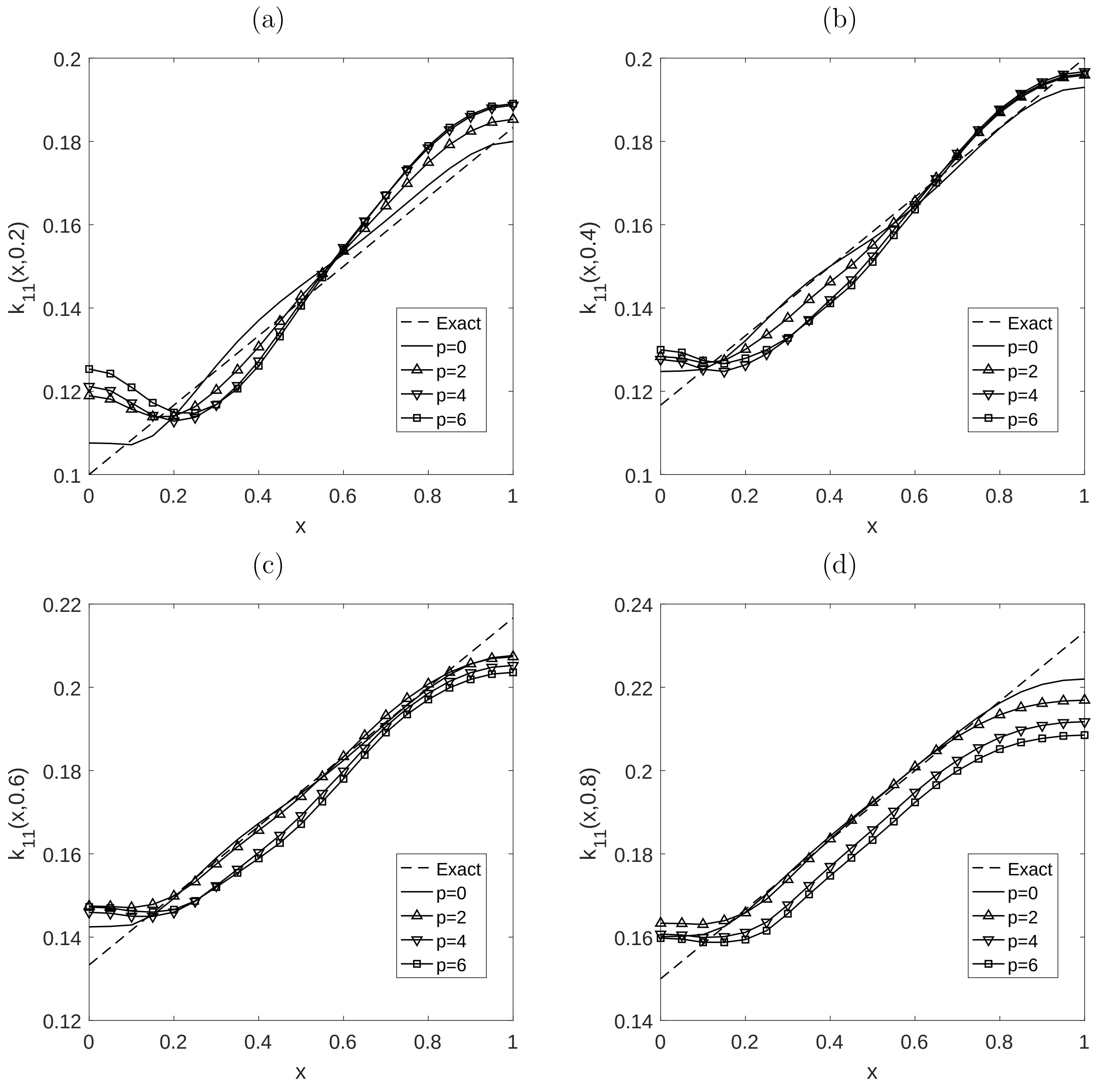

Figure 7: The exact (73) and numerical thermal conductivity component $k_{11}(x, y)$ obtained using the Sobolev $W^{1,2}$-gradient with the initial guess (76) at locations (a) $y = 0.2$, (b) $y = 0.4$, (c) $y = 0.6$ and (d) $y = 0.8$, for $p \in \{0, 2, 4, 6\}$ noise, for Example 2.

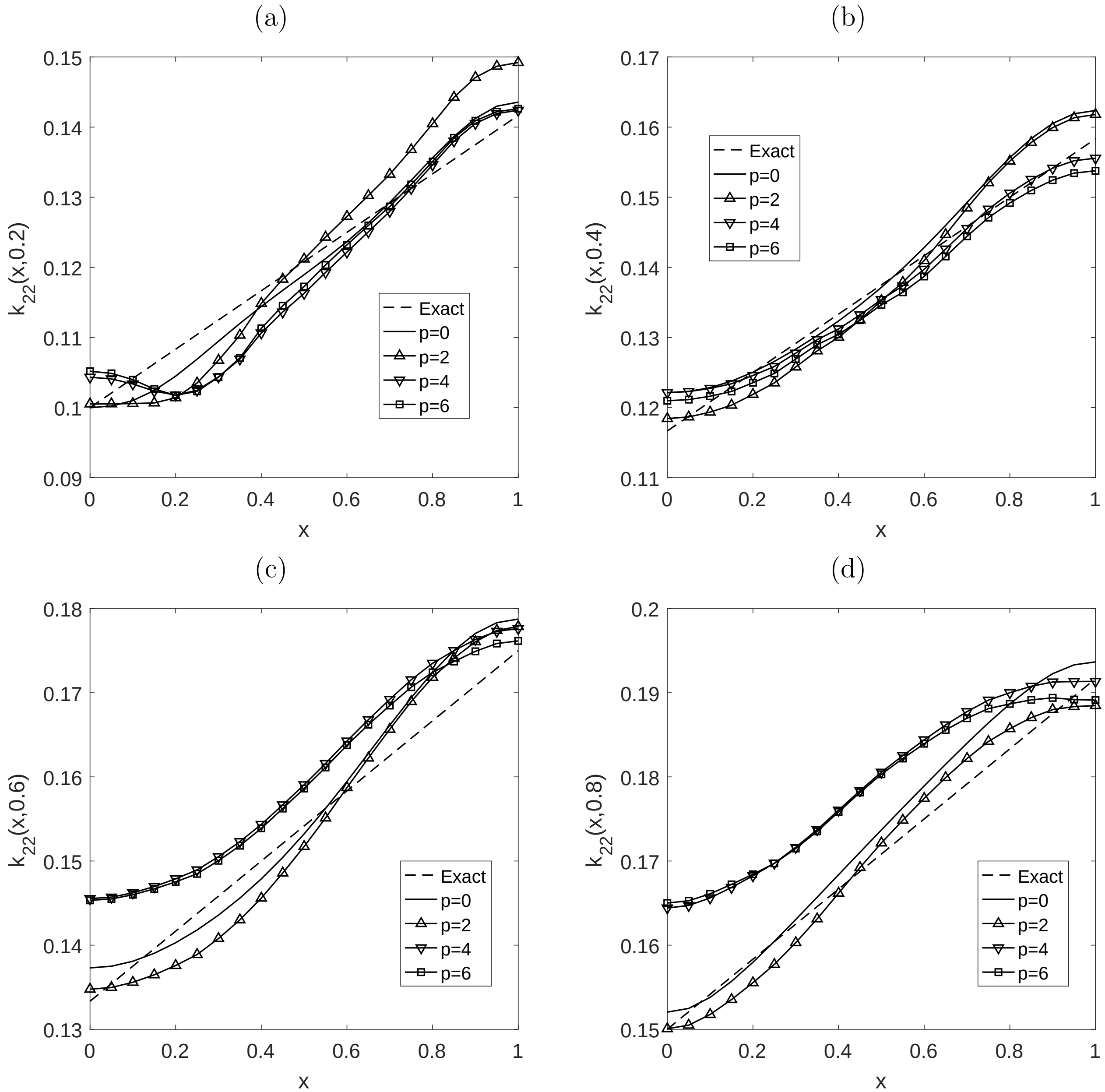

Figure 8: The exact (74) and numerical thermal conductivity component $k_{22}(x, y)$ obtained using the Sobolev $W^{1,2}$-gradient with the initial guess (76) at locations (a) $y = 0.2$, (b) $y = 0.4$, (c) $y = 0.6$ and (d) $y = 0.8$, for $p \in \{0, 2, 4, 6\}$ noise, for Example 2.