

A Data Assimilation Approach to Coefficient Identification

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Abstract

The thermal conductivity properties of a material can be determined experimentally by using temperature measurements taken at specified locations inside the material. We examine a situation where the properties of a (previously known) material changed locally. Mathematically we aim to find the coefficient $k(x)$ in the stationary heat equation $(kT_x)_x = 0$; under the assumption that the function $k(x)$ can be parametrized using only a few degrees of freedom.

The coefficient identification problem is solved using a least squares approach; where the (non-linear) control functional is weighted according to the distribution of the measurement locations. Though we only discuss the $1D$ case the ideas extend naturally to $2D$ or $3D$. Experiments demonstrate that the proposed method works well.

1 Introduction

The thermal properties of a material are often difficult to measure accurately without destroying the object of study. Non-invasive techniques for finding material parameters exists, but more commonly measured data is integrated into mathematical models to produce good estimates [4]. Often it is difficult to acquire measurement data and therefore it is important to make as good use as possible of any available information. In the this work we study the problem of

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determining the thermal conductivity of a material from interior temperature measurements. In particular we are interested in the case when the measurement locations are unevenly distributed. Similar coefficient identification problems often appear in applications [7, 8].

The steady state temperature distribution of a material satisfies,

$$(k(x)T_x)_x = 0, \quad \text{for } a < x < b, \quad (1.1)$$

where the thermal conductivity $k(x)$ is a property of the material. We consider the problem of determining the function $k(x)$ based on temperature measurements at certain available locations inside the material. The goal is to make as good use of the available experimental data as possible, and find approximations of both the temperature distribution $T(x)$ and the thermal conductivity $k(x)$.

Suppose we have a set of locations $\mathcal{X} = \{x_i\}$, satisfying $a < x_i < b$, for $i = 1, \dots, n$, where measurements are available. A standard interpolation scheme provides an approximation $T_I(x) \approx T(x)$. Using the interpolant we can determine $k(x)$ by solving an ordinary differential equation $k_x(x)T_x + k(x)T_{xx} = 0$, with the (known) temperature distribution acting as a coefficient. This type of numerical scheme has been studied previously, see [5, 6, 9, 1], where error estimates and experimental results are reported. Note that since $k(x)T_x(x)$ is constant, for $a < x < b$, and we use linear interpolation to obtain $T_I(x)$, then the reconstructed thermal conductivity is piecewise constant.

In this work we attempt to improve on the results obtained by using an interpolation scheme, and suggest an approach that allows the simultaneous determination of $T(x)$ and $k(x)$. Let $T_I(x)$ be the linear interpolant and consider the minimization problem,

$$\min_V \|V(x) - T_I(x)\|_{L^2(a,b)}, \quad (1.2)$$

where,

$$(k(x)V_x)_x = 0, \quad V(a) = A, \quad V(b) = B.$$

The parameters to determine during the minimization process are the boundary conditions A , B , and the unknown thermal conductivity $k(x)$. A similar technique was applied to a source term identification problem in [3], see also [11], and [2].

Furthermore suppose a material with known thermal properties has been subject to environmental influence that cause the thermal conductivity to change locally, and we are interested in finding the region where the material changes has taken place. A model of this situation is,

$$k(x) = \begin{cases} \kappa, & \alpha < x < \beta, \\ 1, & \text{otherwise,} \end{cases} \quad (1.3)$$

The parameters that determine $V(x)$ are A , B , κ , and also $a < \alpha < \beta < b$.

The disposition of the paper is as follows. In Section 2 we reconstruct $k(x)$ using the linear interpolation. In Section 3 we discuss the minimization problem (1.2) in detail. Numerical experiments are presented in Section 4. Finally a discussion of our results and a few conclusions are given in Section 5.

2 Linear interpolation and coefficient identification

Suppose we have collected temperature data on the set \mathcal{X} , i.e. we have measurements, $T_\delta(x_i) = T(x_i) + \delta_i$, $i = 1, \dots, n$, where $|\delta_i| < \delta$ are the measurement errors. Generally only the upper bound δ is known. In this section we discuss the use of linear interpolation for determining the thermal conductivity $k(x)$.

As previously mentioned the method is based on the idea that, since $T(x)$ satisfies (1.1), the heat-flux $k(x)T_x(x)$ is a constant. Furthermore we assume that, at least, the first two measurement points satisfies $x_1 < x_2 < \alpha$ so that, according to the model (1.3), $k(x_1) = k(x_2) = 1$. We approximate $T(x)$ by a piecewise linear function $T_I(x)$, such that $T_I(x_i) = T_\delta(x_i)$. Differentiating $T_I(x)$ on each subinterval (x_i, x_{i+1}) we obtain $k(x)$.

The coefficient identification problem is ill-posed in the sense that small measurement errors may be magnified during the computations and destroy the numerical solution. However, for our case, the ill-posedness is not severe and in practice problems with realistic noise levels can be solved.

The procedure is illustrated in Figure 2.1, where a data set consisting of $n=15$ temperature measurements was used for determining both T_I and $k(x)$. The simulated measurements included normally distributed random noise with variance $\delta = 10^{-2}$. The coefficient $k(x)$ was reconstructed by assuming that $k(x)=1$ for $x \in [0, 2] \cup [0.8, 1]$, and the constant kT_x was computed as a mean value.

As seen in Figure 2.1 the method, though simple and robust, suffers from several limitations. First we need fairly well spread out measurement points to obtain a good solution. Also we cannot hope to find the interval (α, β) , where the thermal conductivity changed, more accurately than placing α and β in an interval (x_i, x_{i+1}) , i.e. between two measurement points. Furthermore, additional measurements in one small region of the material does not improve the accuracy of the reconstruction as a whole.

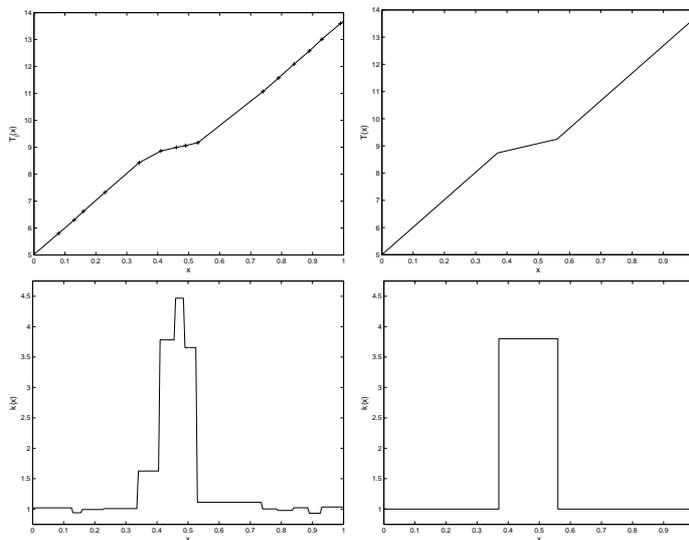


Figure 2.1: The linear interpolant $T_I(x)$ obtained using $n = 15$ measurements (top,left) and the exact solution $T(x)$ (top,right) are displayed. Also the approximation of $k(x)$ obtained by differentiating $T_I(x)$ (bottom,left) and the exact thermal conductivity for this test case (bottom,right) are presented.

3 Optimal model fitting

In this section we discuss the minimization problem (1.2). Clearly, since $V(x)$ satisfies,

$$(k(x)V_x)_x = 0, \quad a < x < b, \quad V(a) = A, \quad V(b) = B, \quad (3.1)$$

where,

$$k(x) = \begin{cases} \kappa, & \alpha < x < \beta, \\ 1, & \text{otherwise.} \end{cases} \quad (3.2)$$

The objective is to find the optimal parameter values, or vector $u = (A, B, \alpha, \beta, \kappa)^T$. Let $\mathcal{X} = \{x_1, \dots, x_n\}$ be the set of measurement points and $T_I(x)$ be the linear interpolant as previously. We introduce the control functional,

$$J(u) = \|V(x) - T_I(x)\|_{L^2(a,b)}, \quad (3.3)$$

where $V(x)$ is the solution of (3.1)–(3.2) defined by the parameter vector u . Thus the coefficient identification problem is replaced by a non-linear least squares problem.

In this work we minimize $J(u)$ numerically as follows. First select an equidistant computational grid $a = z_1 < z_2 < \dots < z_N = b$, and denote by V and T_I the

discretizations,

$$V = (V(z_1), \dots, V(z_N))^T, \quad \text{and,} \quad T_I = (T_I(z_1), \dots, T_I(z_N))^T.$$

The above minimization problem is then approximated by the non-linear least squares problem,

$$\min_u \bar{J}(u), \quad \bar{J}(u) = \|V(u) - T_I\|_2. \quad (3.4)$$

In [10] Landweber iterations were used for solving a similar least squares problem, also related to coefficient identification in PDEs. Here we instead use the Gauss-Newton method to find the optimal parameter values more efficiently. For our problem, the temperature distribution $V(x)$ is parametrized by the 5 parameters in the vector u the Jacobian matrix $F = \partial V / \partial u \in \mathbb{R}^{N \times 5}$, can be computed numerically by finite differences. The Gauss-Newton method for (3.4) can briefly be described as,

$$F(u_n) s_n = -(T_I - V(u_n)), \quad u_{n+1} = u_n + s_n.$$

In our experiments we use a relative tolerance $\|s_n\|_2 / \|u_n\|_2 < 10^{-8}$ as a stopping criterion.

Remark 3.1 By selecting the computational grid $\{z_i\}$ equal to the measurement locations \mathcal{X} we obtain a regular (non-linear) least squares problem. Our motivation for choosing a larger computational grid, and using the linear interpolant $T_I(x)$, is that we obtain a weighted least squares problem, where each measurement point is weighted depending the distance to other measurement locations. This improves the stability of the method. \square

4 Numerical Experiments

In this section we discuss different case studies. We treat the cases with evenly spread as well as unevenly distributed data. For all tests, we choose a computational grid of size $N = 500$. This ensures that the discretization errors are small.

The tests were carried out as follows: First, we selected appropriate values for the parameter vector u , and by solving the direct problem (1.2), evaluating the solution $T(x)$ at the points \mathcal{X} , and adding normally distributed noise, we created simulated measurements \mathcal{Y} . For the coefficient reconstruction we use the data $\{\mathcal{X}, \mathcal{Y}\}$ to find a linear interpolant T_I which is then evaluated on the computational grid z . The functional,

$$\bar{J}(u)^2 = \sum_{i=1}^N |V(z_i) - T_I(z_i)|^2,$$

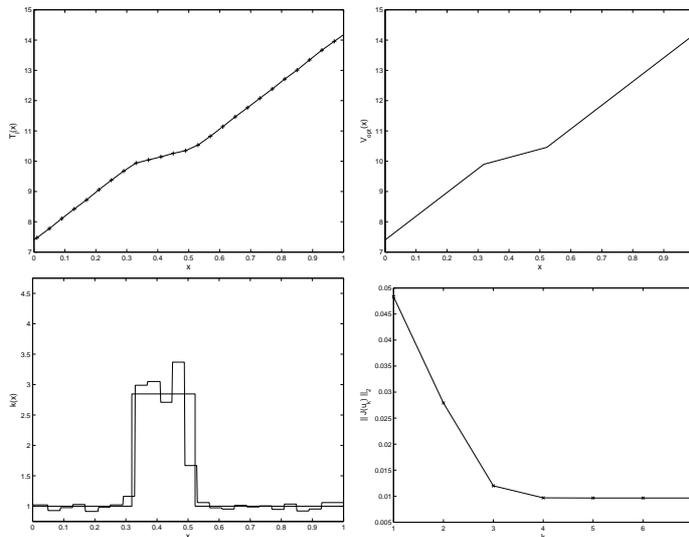


Figure 4.1: Measurements at evenly distributed points are used to find the interpolant $T_I(x)$ (top,left). The temperature distribution $V(x)$ that minimize $J(u)$ (top,right). Also we display both the coefficient $k(x)$ obtained by differentiating T_I and by minimizing $J(u)$ (bottom,left). The convergence history for the Gauss-Newton iterations are also presented (bottom,right).

is then minimized using the Gauss-newton method. Derivatives $\partial V/\partial u$ are computed using central differences. The minimization procedure is not very sensitive with respect to the initial guess u_0 .

For the first experiment, we selected an exact coefficient $k(x)$ and $n=25$ evenly distributed measurement points \mathcal{X} . The experiment is illustrated in Figure 4.1. The exact and reconstructed coefficients $k(x)$ match well. As seen the Gauss-Newton iteration converges rapidly.

For the second experiment, we chose $n=26$ unevenly distributed measurement points. The results are displayed in Figure 4.2. Since the set \mathcal{X} is unevenly distributed the differentiation procedure fails to reconstruct $k(x)$ accurately. However the minimization still give the good result. Again the Gauss-Newton converges in just a few iterations.

Lastly, for the third experiment, we select a function $k(x)$ that isn't an exact step function. Thus the model (1.3) is only approximate. We use $n=21$ evenly distributed measurements to reconstruct $k(x)$. The experiment is presented in Figure 4.3. Note that differentiating T_I does not give a good reconstruction. However, the minimization procedure is stable and give good results.

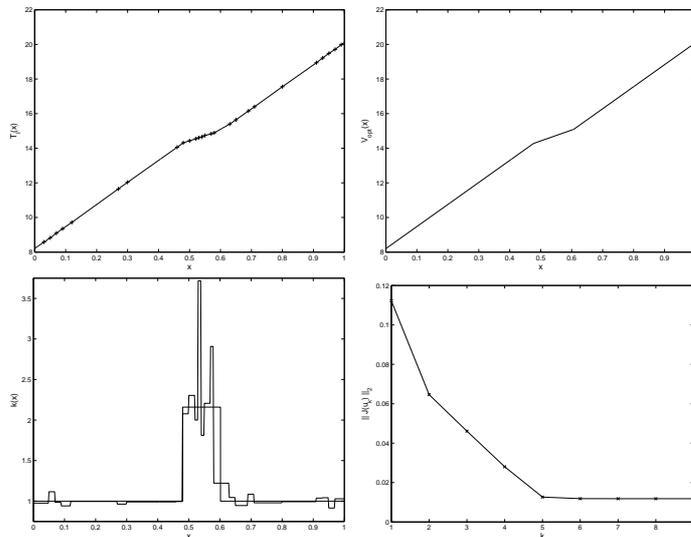


Figure 4.2: Experiment using unevenly distributed measurements. We show the interpolant $T_I(x)$ (top,left) and the temperature distribution $V(x)$ that minimize $J(u)$ (top,right). Also we display both the coefficient $k(x)$ obtained by differentiating T_I and by minimizing $J(u)$ (bottom,left). The convergence history for the Gauss-Newton iterations are also presented (bottom,right).

5 Concluding remarks

In this paper we have investigated a method for finding the thermal conductivity of a material based on temperature data at certain locations inside the material. The proposed method is based on a parametrization of the solution of the underlying differential equation. The optimal parameter values are then computed numerically by minimizing a certain functional, using the Gauss-Newton method. The resulting scheme is rather robust, efficient, and good approximations of the model parameters are obtained.

We have assumed that the thermal conductivity is known, except for an interval inside the material where physical, or chemical, changes have occurred. Hence the function $k(x)$ can be parametrized by the three parameters α , β , and κ . For our scheme to work it is essential that $k(x)$ can be parametrized using relatively few degrees of freedom. However, more general functions $k(x)$ can be dealt with. For instance suppose $k(x) = 1$ near the boundaries $x = a$ and $x = b$ and smooth

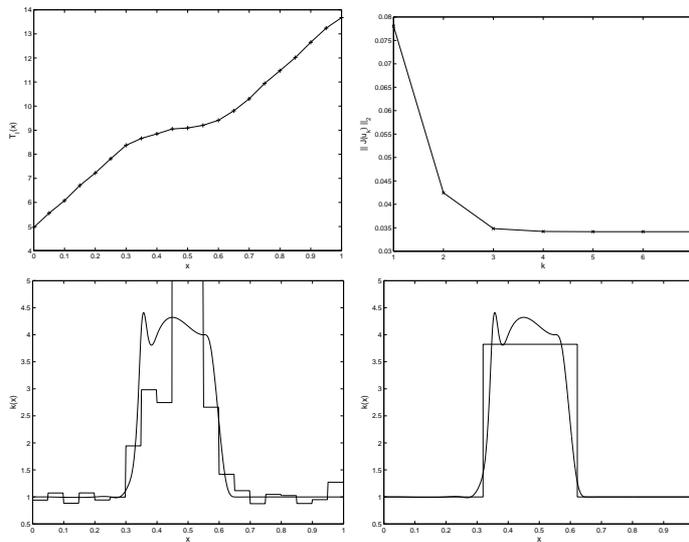


Figure 4.3: Experiment with an inexact coefficient model and evenly distributed measurements. We display the interpolant $T_I(x)$ (top, left) and the resulting convergence history for the Gauss-Newton method (top, right). Also, the coefficient $k(x)$ obtained by differentiating T_I (bottom, left) and by minimizing $J(u)$ (bottom, right). In both cases the reconstruction is compared with the exact function $k(x)$.

inside the material. Then we can parametrize,

$$k(x) = 1 + \sum_{k=1}^p c_k B(x - x_k),$$

where $B(x - x_k)$ are suitable B -spline basis functions, with support inside the interval (a, b) . Using B -splines additional conditions, of various types, on the unknown thermal conductivity $k(x)$ can be parametrized efficiently.

Though in this work we have restricted ourselves to a one dimensional case where the solution can be computed analytically the scheme extends naturally to two or three dimensional problems. For instance,

$$\nabla(k\nabla T) = 0,$$

or time dependent equations,

$$T_t = (k(x)T_x)_x.$$

If the coefficient $k(x)$ and the boundary conditions can be parametrized using only a small number of parameters then we can compute the Jacobian matrix

needed for the Gauss-Newton iteration by solving appropriate boundary value problems. This is a topic that we will investigate further in upcoming papers.

References

- [1] V. T. Borukhov and P. N. Vabishchevich. Numerical solution of the inverse problem of reconstructing a distributed right-hand side of a parabolic equation. *Comput. Phys. Comm.*, 126(1-2):32–36, 2000. Modern trends in computational physics (Dubna, 1998).
- [2] Mehdi Dehghan. Determination of a control function in three-dimensional parabolic equations. *Math. Comput. Simulation*, 61(2):89–100, 2003.
- [3] Zui-Cha Deng, Jian-Ning Yu, and Liu Yang. Optimization method for an evolutionary type inverse heat conduction problem. *J. Phys. A: Math. Theor.*, 41(3), 2008.
- [4] D. Hinestroza. Identification of transmissivity coefficients by mollification techniques. II. n -dimensional elliptic problems. *Comput. Math. Appl.*, 30(1):11–30, 1995.
- [5] Doris Hinestroza and Diego A. Murio. Recovery of the transient heat transfer coefficient in the nonlinear boundary value problem for the heat equation. *Comput. Math. Appl.*, 25(5):101–111, 1993.
- [6] Doris Hinestrozas and Diego A. Murio. Identification of transmissivity coefficients by mollification techniques. I. One-dimensional elliptic and parabolic problems. *Comput. Math. Appl.*, 25(8):59–79, 1993.
- [7] V. Isakov and S. Kindermann. Identification of the diffusion coefficient in a one-dimensional parabolic equation. *Inverse Problems*, 16:665–680, 2000.
- [8] D. Lesnic. The determination of the thermal properties of a heat conductor in a nonlinear heat conduction problem. *Z. Angew. Math. Phys.*, 53(2):175–196, 2002.
- [9] C. E. Mejía and D. A. Murio. Mollified hyperbolic method for coefficient identification problems. *Computers Math. Applic.*, 26(5):1–12, 1993.
- [10] Liu Yang, Zui-Cha Deng, Jian-Ning Yu, and Guan-Wei Luo. Two regularization strategies for an evolutionary type inverse heat source problem. *J. Phys. A: Math. Theor.*, 42(36), 2009.
- [11] Zh. Yi and D. A. Murio. Source term identification in 1-D IHCP. *Comput. Math. Appl.*, 47(12):1921–1933, 2004.