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SOME NUMERICAL RESULTS ON THE PARAMETER IDENTIFICATION PROBLEM FOR THE HEAT CONDUCTION EQUATION

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1. Introduction

The parameter identification problem is known also as the inverse problem.

Some experimental investigations are described in [1] and one can find theoretical results by A. D. Iskenderov, R. J. Lermit, J. W. Mosevich, B. F. Jones, A. V. Balakrishnan, G. I. Marchuk and others. There exist many different ways of approach.

Suppose the values of the solution of the heat conduction equation have been measured at discrete points in time and space (discrete observation). The continuous dependence of the undetermined coefficients on the data and the region is proven for this partial differential equation.

The problem of determination or identification of the parameters of a solid arises in course of the development of new solids in the glass, ceramic or steel industry.

2. The ordinary differential equation as an illustration

The simple and well known growth problem of a population is defined by the ordinary differential equation

$$y'(t) = cy(t), \quad y(0) = y_0 > 0, \quad 0 \leqslant t \leqslant T, \tag{1}$$

where a sequence $\{y_i\}_{i=0}^{N}$ of measured data (an observed solution) $y_i = y(t_i)$, $0 = t_0 < t_1 < \ldots < t_N = T$, is given and the constant c is unknown. The solution of (1) is

$$y(t) = y_0 \exp(ct). \tag{2}$$

First let us discuss some possibilities of evaluating c:

1. The analytic solution for the value of c is

$$c = c(t) = \frac{1}{t} \ln \frac{y(t)}{y_0}. \tag{3}$$

Assume a specific value for t; we ignore many other points because of the general situation $c(t_i) \neq c(t_j)$ for $i \neq j$.

2. The assumption

$$c = \frac{y'(t)}{y(t)} \approx \frac{y(t_{i+1}) - y(t_i)}{\Delta t_i \cdot y(t_i)} \tag{4}$$

is also very poor since numerical differentiation is required. We must again choose a specific t.

3. The following consideration based on the equivalent integral equation

$$y(t) = y_0 + c \int_0^t y(x)\,dx \tag{5}$$

supplies a better approximation

$$c = \frac{y(t) - y_0}{\int_0^t y(x)\,dx}. \tag{6}$$

4. The best approximation for c based on all values y_i is obtained by the following

$$y' = cy,$$

$$\int_0^t y'(x)\,dx = c \int_0^t y(x)\,dx,$$

$$\int_0^T \big(y(t) - y_0\big)\,dt = \int_0^T \int_0^t y'(x)\,dx\,dt = c \int_0^T \int_0^t y(x)\,dx\,dt$$

$$= c \int_0^T (T - x)\, y(x)\,dx,$$

$$c = \int_0^T \big(y(t) - y_0\big)\,dt \Big/ \int_0^T (T - t)\, y(t)\,dt, \tag{7}$$

which requires more computing expense.

All these cases show the difficulties arising in the solution of this simple inverse problem.

3. The heat conduction equation

Let us consider a solid given as a full infinite cylinder, and assume that we have the possibility to measure the temperature $\bar{T}(x, t)$ at points $(\bar{r}_i, \bar{t}_j)$ belonging to the set

$$G_{\rm mes} = \{(\bar{r}_i, \bar{t}_j):\ i = 0, 1, \ldots, r_m,\ 0 \leqslant \bar{r}_0 < \bar{r}_1 < \ldots < \bar{r}_{r_m};\ j = 0, 1, \ldots, t_m,\ \bar{t}_j = j\cdot Z/t_m \text{ (equidistant)},\ Z \text{ — whole time of measurement}\}. \tag{8}$$

The solid is homogeneous, isotropic and without heat sources.

We consider the temperature as a solution of the one-dimensional heat conduction equation in an infinite cylinder with the radius $R = \bar{r}_{r_m}$. This parabolic initial-boundary value problem has the form

$$(c\varrho)(T)\frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\lambda(T)\frac{\partial T}{\partial r}\right) \tag{9}$$

in the bounded domain $G = \{(r, t):\ 0 < r < R,\ 0 < t \leqslant Z\} \subset \boldsymbol{R}^2$ with

$$T(r, 0) = u_0(r), \quad 0 \leqslant r \leqslant R \quad \text{(initial condition)}, \tag{10}$$

$$\left.\frac{\partial T}{\partial r}\right|_{r=0} = 0, \quad T(R, t) = \varphi_1(t), \qquad t > 0 \quad \text{(boundary condition)}, \tag{11}$$

where the coefficients, the heat conductivity λ, the density ϱ, the specific heat c and the heat capacity per unit volume $c\varrho$ are positive. Either $c\varrho$ or λ is the unknown function of T.

4. The identification algorithm

Analyzing this problem numerically, we assume the following step algorithm:

1. Approximation to the I.C. $u_0(r)$ using the values $\bar{T}(\bar{r}_i, 0)$:
— manual, e.g. with cubic splines,
— by the Newton interpolation polynomial of degree $k = r_m \leqslant 4$,

– by the least squares method using polynomials of degree $k \leqslant \min(4, r_m)$.

2. Approximation to the B.C. $\varphi_1(t)$ using the values $\overline{T}(R, t_j)$:
– manual,
– by the piecewise-linear function (a polygonal line) through the values $\overline{T}(R, t_j)$,
– by the least squares method using polynomials (of degree $k \leqslant \min(4, t_m)$) or the exponential function $(b \cdot \exp(dt))$.

3. Solution of (9)–(11) with use of a finite difference method assuming the equidistant mesh

$$G_h = \{(r_i, t_j): r_i = i \cdot h,\ h = R/N_r \text{ spatial step size}; \quad t_j = j \cdot \tau,\ \tau = Z/N_t \text{ temporal step size}\} \tag{12}$$

such that N_t/t_m and $(\bar{r}_{i+1} - \bar{r}_i)/h$ are integers. Then we have $G_{\text{mes}} \subset G_h \subset \bar{G}$.
We seek either $c\varrho$ or λ in the form

$$\sum_{i=1}^{n} a_i T^{i-1}, \quad \text{where } n \leqslant 7. \tag{13}$$

The following difference schemes are possible:
– explicit method,
– implicit linearized method (chase method; progonka (Russ.)),
– implicit iterative method,
– Crank–Nicolson linearized,
– Crank–Nicolson iterative.

4. Computation of the functional

$$E(a_1, a_2, \ldots, a_n) = \sum_{i=0}^{r_m} \sum_{j=0}^{t_m} \left(\overline{T}(\bar{r}_i, \bar{t}_j) - T(\bar{r}_i, \bar{t}_j)\right)^2 \tag{14}$$

and its minimization by a gradient-like method

$$a^{(m+1)} = a^{(m)} + p_m \cdot s^{(m)}, \quad m = 0, 1, \ldots; \ a^{(0)} \text{ given}, \tag{15}$$

with the finite difference approximation of the Jacobian matrix, i.e.

$$s^{(m)} = -JE(a^{(m)}) \quad \text{(steepest descent step)}$$

or the Hessian matrix, i.e.

$$s^{(m)} = -H^{-1} JE(a^{(m)}) \quad \text{(Newton step)}.$$

There exists a computer test program in PL/1 and ALGOL 1204 with some additional refinements.

5. Numerical examples

We have tested the algorithm on the ES 1040 computer in double precision on several test problems of varying character and difficulty.

Test problem 1. For a cylindrical solid we have measured 6 different temperature fields $\bar{T}_i$ by cooling and/or heating, with $u_0(r)$ = constant. The parameters are given in Table 1:

Table 1

	r_m	t_m	$R = \bar{r}_{r_m}$ (m)	Z (h)	$\bar{r}_0$	$\bar{r}_1$	$\bar{r}_2$	$\bar{r}_3$
$\bar{T}_1, \bar{T}_2$	3	60	.030	1/2	.014	.023	.026	.03
$\bar{T}_3, \bar{T}_4, \bar{T}_5$	3	40	.030	1/3	.014	.023	.026	.03
$\bar{T}_6$	2	30	.030	1/4	.014	,026	.030	

The coefficient $c\varrho$ is equal to 720 and we seek the constant function $\lambda = a_1$. The algorithm applies the least squares method using polynomials of degree $k = 0$ for $u_0(r)$, the polygonal lines for $\varphi_1(t)$ and the difference method "C–N linearized" with the grid size $30 \times t_m$. For each example the minimization process is convergent for arbitrary nonnegative start point $a_1^{(0)}$ and computes 6 values of a_1 and the average deviation $D = \mathrm{sqrt}\left(\frac{1}{(r_m+1)(t_m+1)} \cdot E(a_1)\right)$, as shown in Table 2:

Table 2

	$\bar{T}_1$	$\bar{T}_2$	$\bar{T}_3$	$\bar{T}_4$	$\bar{T}_5$	$\bar{T}_6$	first 1/2 part $\bar{T}_2$
a_1	1.172	1.264	1.186	1.258	1.354	1.213	1.240
D (°)	2.2	6.4	1.9	1.4	1.2	1.0	8.3

All measured temperatures belong to the interval (83°, 441°).

Test problem 2. A temperature field $\bar{T}$ was generated by the program itself and then we have tried to identify the values carrying out the minimization (15) with different start vectors $a^{(0)}$.

The parameters and data for generation are

$$
(16)\qquad
\begin{array}{ll}
R = \bar{r}_{r_m} = 0.030\,\mathrm{m}, & c\varrho = 720, \\
 & \lambda = 1.2, \\
Z = 0.25\,\mathrm{h}, & u_0(r) = 342, \\
r_m = 3, & \varphi_1(t) = 342\cdot\exp(-t), \\
t_m = 30, & \bar{r}_0 = 0, \\
N_r = 10, & \bar{r}_1 = 0.015, \\
N_t = 30, & \bar{r}_2 = 0.024, \\
\text{“C–N linearized”}, & \bar{r}_3 = 0.030.
\end{array}
$$

The function $\lambda = 1.2$ is our unknown.

Variant 1: $n = 1$. The algorithm is convergent for every start point $a_1^{(0)} \geqslant 0$ and also for $a_1^{(0)} < 0$, while we do not compute number overflow, see Fig. 1. The numerical investigation underlines the existence

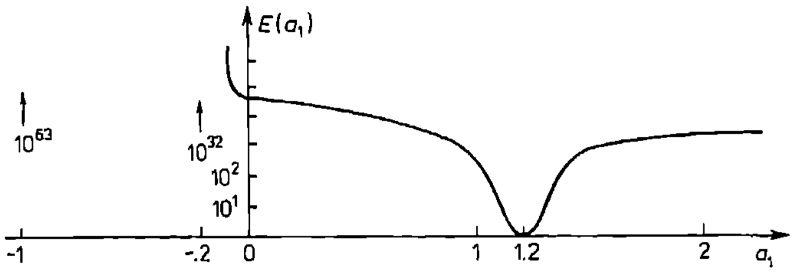

Fig. 1. The function $E(a_1)$

and uniqueness of solution (a constant positive value) and the convergence of minimization process to this constant.

Variant 2: $n = 2$. Figures 2 and 3 show the domain of convergence of the minimization algorithm lying above the curve

$$a_2 = -3\cdot 10^{-3}a_1 - 10^{-3}.$$

In other domains the coefficient $\lambda = a_1 + a_2T$, $0 \leqslant T \leqslant 342$, is very negative, and hence not allowed in equation (9). This is also the case of a great deal of extrema. Choosing a start vector $a^{(0)}$ in this domain we cannot expect, in general, a descent process to the absolute minimum.

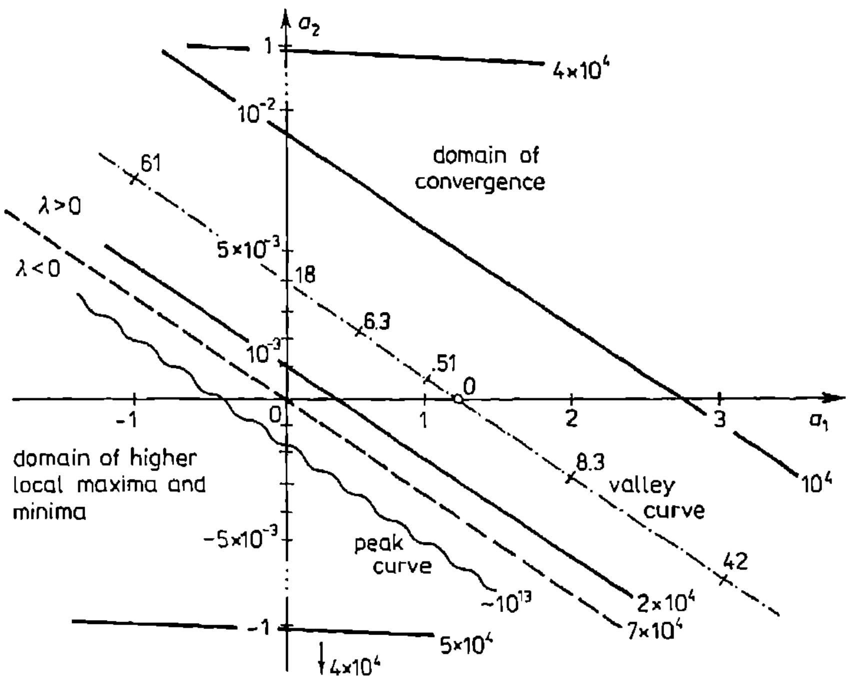

Fig. 2. Level curves of the function $E(a_1, a_2)$

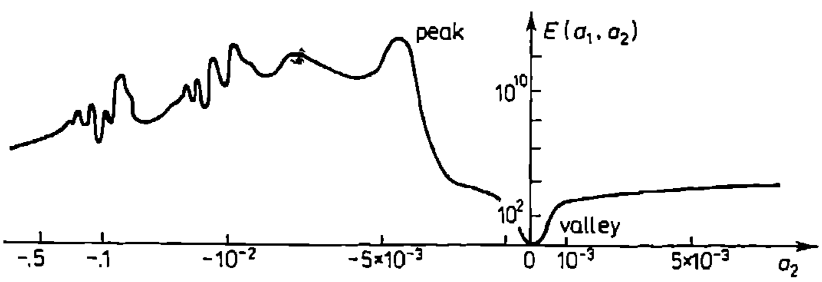

Fig. 3. The function $E(a_1, a_2)$ with the constant component $a_1 = 1.2$

The examples given in Table 3 show the good quality and performance of the procedure.

For the computation of the value $E(a)$ we must always solve the problem (9)–(11), (16) approximatively. The computing time is about 120 sec and belongs for all tests to the interval $F(1, 1.2)$, where F is the last number in the 4th column of Table 3, here $86+2\cdot9 = 104$.

Table 4 shows that we can obtain convergence in spite of an unfavourable choice of the start vector. In the second part of this table we illustrate the minimization process if a_1 = constant. The algorithm is very slow if the component a_2 lies far away from the valley curve in the positive direction.

Also in this case the existence and uniqueness seem to be guaranteed under additional conditions on the coefficient functions, I.C. and/or B.C.

Table 3

N	$\lambda = a_1$ +	$a_2 \cdot T$	F	$E(a)$
0	.5	.0	1	1.16E4
1	.5000 2030	.0064 6648	5	7.74E3
2	−16.5988 271	.0603 4697	20	4.77E3
3	−13.0407 149	.0462 3392	31	2.41E3
4	−13.0407 127	.0468 3369	43	2.37E3
5	− .9663 8062	.0061 9034	57	4.40E2
6	−2.0544 6040	.0103 4211	66	1.43E2
7	1.1803 6579	.0000 7479	77	1.80E−1
8	1.2023 3812	−.0000 0741	82	7.27E−5
9	1.2007 6385	−.0000 0230	$86 + 2 \cdot 9$	3.05E−5

N – number of iteration, F – number of evaluations of the function $E(a)$

Table 4

N	$\lambda = a_1$ +	$a_2 \cdot T$	F	$E(a)$
0	1.2	−.01	1	3.25E11
1	1.2233 2787	.0202 4551	5	2.68E4
2	1.2420 2062	.0058 2810	15	1.14E4
...				
4	8.7814 7573	−.0239 4664	36	8.12E2
...				
6	4.0604 7108	−.0093 8961	68	2.46E2
7	1.4583 2575	−.0007 9787	79	1.67E0
8	1.2065 5343	−.0000 2157	85	1.07E−3
9	1.1988 8587	.0000 0335	90	6.47E−5
...				
18	1.2009 0873	−.0000 0294	128	1.23E−5
...				
177	1.2007 5754	−.0000 0242	3551	7.37E−6
0	1.2	−.01	1	3.25E11
1	1.2	.0281 9660	5	3.02E4
2	1.2	.0265 6007	17	2.97E4
3	1.2	.0197 0204	21	2.02E4

Variant 3: $n = 3$. We obtain no convergence (or, maybe, very slow convergence) also for $a^{(0)} \approx 1.2$, as can be shown not only by the following examples.

Table 5

N	$\lambda = a_1$	$+ \quad a_2 \cdot T +$	$a_3 \cdot T^2$	F	$E(a)$
0	1.15	.0	.0	1	3.17E1
...					
21	1.1226 8605	.0004 9861	−.0000 0080	248	1.72E−4
...					
26	1.1226 8600	.0004 9861	−.0000 0080	434	1.72E−4
0	1.3	.0	.0	1	1.11E2
...					
62	.9980 1268	.0005 8158	.0000 0023	1381	7.49E−1
...					
105	1.2314 4216	−.0002 0278	.0000 0033	2133	2.85E−5

6. Conclusion and discussion

In order to recognize the specific nature of the identification problem it would be desirable to answer some open problems and to aim at further improvements of the algorithm. These are

1. For what cases and under what conditions is the existence and uniqueness of the solution provided?

2. What can be said about the size of the set of measured values $\overline{T}$?

3. What is the influence of perturbations in the field $\overline{T}$ on the solution?

4. Among functions of what form are we to seek the coefficient functions $c\varrho$ or λ?

5. Addition of a regularization term (penalty function) and a corrector term to our functional in order
   - to obtain a convex function and smoothing effect on the solution,
   - to stick to the admissible domain of the unknown coefficient.

6. Choice of one or more functionals E.

This is to point out the necessity of continuation of further systematical theoretical and practical investigations.

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