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A.R. Baitureyeva[1,*], B. Rysbaiuly[2]

[1]Al-Farabi Kazakh National University, 71 Al-Farabi Ave., 050040, Almaty, Kazakhstan
[2]Astana IT University, Mangilik El avenue, 55/11, 010000, Astana, Kazakhstan
*e-mail: baitureyeva.aiymzhan@gmail.com

Inverse problem for determining the coefficient in the heat conduction equation

Abstract. This paper considers the inverse problem of determining the thermal conductivity coefficient in the heat equation. The objective of this study is to determine the unknown coefficient based on measured boundary temperature data over time. The governing equation is a parabolic partial differential equation that describes the heat transfer process, with the unknown thermal conductivity playing a decisive role in the solution. The inverse problem is formulated as an optimization problem, in which the discrepancy between the simulated temperature distribution and the experimental data is minimized. Numerical modeling methods were used to solve the problem, including the tridiagonal matrix algorithm (Thomas algorithm) for discretizing the heat equation. The optimization process was performed using gradient methods, where the adjoint problem was used to efficiently calculate the gradient of the objective function with respect to the thermal conductivity coefficient. The results demonstrated acceptable accuracy in reconstructing the coefficient. Different parameters for the reduction factor in the gradient method were also considered. These findings are important for applications in fields such as materials science, geophysics, and engineering, where accurate estimation of thermal properties is essential.
Key words: inverse problem, heat transfer, adjoint problem, thermal conductivity coefficient, numerical modeling.

1. Introduction

The accurate determination of thermal properties, particularly the thermal conductivity coefficient, is important in various scientific and engineering fields, such as materials science, geophysics, and energy systems engineering. Thermal conductivity is a critical parameter that characterizes the ability of a material to conduct heat and is crucial for designing efficient thermal management systems, improving material performance, and understanding heat transfer mechanisms in different environments [1]. Consequently, accurate estimation of thermal conductivity is fundamental to achieving optimal performance in applications ranging from industrial processes to environmental modeling.

The heat conduction equation, a parabolic partial differential equation (PDE), governs the distribution of temperature in a given domain over time. This equation has been extensively studied and applied in scenarios involving heat transfer, such as in solids and fluids. Thermal conductivity is one of the most decisive factors influencing heat transfer behavior. However, in many practical situations, the thermal conductivity coefficient is not readily available, either because it is difficult to measure directly or because the material properties change over time or space. In such cases, it becomes necessary to solve an inverse problem to identify the unknown coefficient based on observed temperature data [2].

Inverse problems are inherently more challenging than direct problems. In a direct problem, the governing equations and material parameters are known. In contrast, in an inverse problem, some information – such as material properties like the thermal conductivity coefficient or boundary conditions – is missing, and the goal is to deduce this missing information based on measurements of the system's response, such as boundary or internal temperatures [3] – [8].

In this study, the inverse problem of determining the thermal conductivity coefficient in the heat equation using boundary temperature measurements over time was addressed. In particular, spruce was considered as the main material. Synthetic values at $k = 0.65\ [W\ m^{-1}\ C^{-1}]$ (thermal conductivity coefficient of spruce) were used as experimental measurements. The primary focus is on developing a robust numerical approach to efficiently and accurately estimate the unknown coefficient. Specifically, the inverse problem is formulated to minimize the discrepancy between the simulated temperature distribution and the experimental measurements. This approach enables iterative adjustment of the unknown coefficient to best match the observed data, thus yielding an estimate of the thermal conductivity [9].

The tridiagonal matrix algorithm (Thomas algorithm) was employed for the discretization of the heat equation. The gradient of the objective function with respect to the thermal conductivity coefficient was computed using the adjoint problem, significantly enhancing computational efficiency [10].

Additionally, the influence of descent parameters within the gradient optimization method was explored, focusing on the accuracy and convergence speed of the solution. This step is crucial to ensuring that the optimization process remains stable and that the reconstructed coefficient is as accurate as possible. Numerical experiments were conducted to assess the performance of the proposed method, and the results demonstrated acceptable accuracy in reconstructing the thermal conductivity coefficient.

The findings of this study have significant implications for practical applications where precise thermal property estimation is required. Future work may explore extending this method to more complex scenarios, such as multidimensional heat conduction problems, and incorporating advanced regularization techniques to enhance robustness against measurement errors.

All calculations were performed using Jupyter Lab and implemented in Python using the NumPy and Matplotlib libraries for efficient numerical analysis and data visualization.

2. Mathematical models and methods

The temperature distribution in spatial domain and its variation over time are described by a second-order partial differential equation.

$$\frac{\partial T(x,t)}{\partial t} = k\frac{\partial^2 T(x,t)}{\partial x^2},\ 0 < x < L, 0 < t < T \quad (1)$$

Here $T(x,t)$ is the temperature distribution depending on the coordinate x and time t. Neumann conditions are set at the lateral boundaries of the region:

$$\left.\frac{\partial T}{\partial x}\right|_{x=0} = \left.\frac{\partial T}{\partial x}\right|_{x=L} = 0 \quad (2)$$

Initial condition:

$$T|_{t=0} = f(x), \text{ where } f(x) = 6 \cdot \sin\left(\frac{\pi x}{L}\right) \quad (3)$$

The thermal conductivity coefficient k is unknown and must be determined by solving the inverse problem.

Further, all problems are solved in discrete form. To achieve this, the interval $(0, L)$ is divided into N equal parts with a step size of $\Delta x = \frac{L}{N}$, and the interval $(0, t_{max})$ is divided into m equal parts with a step size of $\Delta t = \frac{t_{max}}{m}$. As a result, a grid domain is formed with a mesh $\omega = \{(x_i, t_j), x_i = i\Delta x, t_j = j\Delta t, i = 0, \ldots, N, j = 0, \ldots, m\}$. At the node (x_i, t_j), the exact values of the functions $T(x_i, t_j)$ are located.

The problem is approached iteratively. Initially, the n-th approximation $k(n)$ is specified. The next approximation $k(n+1)$ for the subsequent iteration is obtained by minimizing the functional:

$$I = \sum_{j=0}^{m-1} \left(T_N^{j+1} - T_{exp}^{j+1}\right)^2 \Delta t \to min,$$

$$j = 0, \dots, m-1 \tag{4}$$

Where T_N^{j+1} is the temperature at the right boundary obtained by the numerical solution, and T_{exp}^{j+1} is the experimentally measured value on the surface of the spruce.

All calculations are performed in the domain $\omega = (0, L) \times (0, T)$, where $L = 1, T = 1$. When the exact value of k is found, the numerical solution yields accurate results, and the value of the functional tends to zero. To minimize I, sensitivity and adjoint problems are formulated [11].

3. Derivation of the sensitivity and adjoint problems

The discrete form of equation (1) is considered as follows:

$$T_{i,\bar{t}}^{j+1} = k\, T_{i,x\bar{x}}^{j+1} \tag{5}$$

Where

$$T_{i,\bar{t}}^{j+1} = \frac{T_i^{j+1} - T_i^j}{\Delta t},$$

$$T_{i,x\bar{x}}^{j+1} = \frac{T_{i+1}^{j+1} - 2T_i^{j+1} + T_{i-1}^{j+1}}{(\Delta x)^2}$$

$\bar{x}, \bar{t}$ mean the backward difference approximation, and x, t denotes the forward difference approximation, respectively.

The delta operator Δ is introduced to represent the difference between two consecutive steps n and $n+1$:

$$\Delta T_i^{j+1} = T_i^{j+1}(n+1) - T_i^{j+1}(n)$$

where $n -$ iteration number. Applying the delta operator to system (1)–(4) yields:

$$\Delta T_{i,\bar{t}}^{j+1} = \Delta\left(k T_{i,x\bar{x}}^{j+1}\right) \tag{6}$$

$$\Delta T_{1,\bar{x}}^{j+1} = 0,\ \Delta T_{N,\bar{x}}^{j+1} = 0 \tag{7}$$

$$\Delta T_i^0 = 0 \tag{8}$$

Subsequently, the adjoint problem is derived from the sensitivity problem (6)–(8).

Equation (6) is multiplied by an arbitrary grid function $\psi_i^j \Delta x \Delta t$ and summed over all grid points.

$$\omega = \left\{(x_i, t_j), x_i = i\Delta x, t_j = j\Delta t, i = = 1, \dots, N-1, j = 0, \dots, m\right\}$$

Then

$$\sum_{i=1}^{N-1} \sum_{j=0}^{m-1} \Delta T_{i,\bar{t}}^{j+1} \psi_i^j \Delta t \Delta x = = \sum_{j=0}^{m-1} \sum_{i=1}^{N-1} \Delta\left(k T_{i,x\bar{x}}^{j+1}\right) \psi_i^j \Delta x \Delta t \tag{9}$$

The formula for summation by parts is derived by considering the following expression:

$$f_i g_i - f_{i-1} g_{i-1} = g_i f_{i,\bar{x}} \Delta x + f_{i-1} g_{i,\bar{x}} \Delta x$$

The final equality is summed over i from k to n:

$$f_n g_n - f_{k-1} g_{k-1} = = \sum_{i=k}^{n} g_i f_{i,\bar{x}} \Delta x + \sum_{i=k}^{n} f_{i-1} g_{i,\bar{x}} \Delta x$$

This resulting equality can be rewritten in the following form:

$$\sum_{i=k}^{n} g_i f_{i,\bar{x}} \Delta x = = f_n g_n - f_{k-1} g_{k-1} - \sum_{i=k}^{n} f_{i-1} g_{i,\bar{x}} \Delta x \tag{10}$$

or in this form:

$$\sum_{i=k}^{n} f_{i-1} g_{i,\bar{x}} \Delta x = f_n g_n - f_{k-1} g_{k-1} - \sum_{i=k}^{n} g_i f_{i,\bar{x}} \Delta x \tag{11}$$

The summation by parts formula (10) is applied to the left-hand side of equation (9) with respect to the variable j:

$$\sum_{i=1}^{N-1}\sum_{j=0}^{m-1}\Delta T_{i,\bar{t}}^{j+1}\,\psi_i^j\Delta t\Delta x=\sum_{i=1}^{N-1}(\Delta T_i^m\psi_i^m-\Delta T_i^0\psi_i^0)\Delta x-\sum_{i=1}^{N-1}\sum_{j=0}^{m-1}\Delta T_i^{j+1}\psi_{i,\bar{t}}^{j+1}\Delta t\Delta x$$

Taking into account the initial conditions (8) and assuming that

$$\psi_i^m=0, i=1,2,\dots,N$$

the following equation is obtained:

$$\sum_{i=1}^{N-1}\sum_{j=0}^{m-1}\Delta T_{i,\bar{t}}^{j+1}\,\psi_i^j\Delta t\Delta x=-\sum_{i=1}^{N-1}\sum_{j=0}^{m-1}\Delta T_i^{j+1}\psi_{i,\bar{t}}^{j+1}\Delta t\Delta x \qquad (12)$$

Applying the summation by parts formula (11), the right-hand side of equation (9) is transformed as follows:

$$\sum_{j=0}^{m-1}\sum_{i=1}^{N-1}\Delta\left(kT_{i,x}^{j+1}\right)_{\bar{x}}\psi_i^j\Delta x\Delta t=$$

$$=\sum_{j=0}^{m-1}\left(\Delta\left(kT_{N,\bar{x}}^{j+1}\right)\psi_N^j-\Delta\left(kT_{1,\bar{x}}^{j+1}\right)\psi_0^j\right)\Delta t-\sum_{j=0}^{m-1}\sum_{i=1}^{N-1}\Delta\left(kT_{i,x}^{j+1}\right)\psi_{i,x}^j\Delta x\Delta t$$

Using the boundary conditions (7):

$$\sum_{j=0}^{m-1}\sum_{i=1}^{N-1}\Delta\left(kT_{i,x}^{j+1}\right)_{\bar{x}}\psi_i^j\Delta x\Delta t=-\sum_{j=0}^{m-1}\sum_{i=1}^{N-1}\Delta\left(kT_{i,x}^{j+1}\right)\psi_{i,x}^j\Delta x\Delta t \qquad (13)$$

Based on (10) and (11), the relation (9) is expressed as:

$$-\sum_{i=1}^{N-1}\sum_{j=0}^{m-1}\Delta T_i^{j+1}\,\psi_{i,\bar{t}}^{j+1}\Delta t\Delta x=-\sum_{j=0}^{m-1}\sum_{i=1}^{N-1}\Delta\left(kT_{i,x}^{j+1}\right)\psi_{i,x}^j\Delta x\Delta t \qquad (14)$$

Using the obvious equality:

$$\Delta(fg)=\Delta f g(n+1)+f(n)\Delta g$$

The equation (14) can be rewritten as follows:

$$-\sum_{i=1}^{N-1}\sum_{j=0}^{m-1}\Delta T_i^{j+1}\,\psi_{i,\bar{t}}^{j+1}\Delta t\Delta x=$$

$$=-\sum_{j=0}^{m-1}\sum_{i=1}^{N-1}\Delta kT_{i,x}^{j+1}(n+1)\,\psi_{i,x}^{j}\Delta x\Delta t-\sum_{j=0}^{m-1}\sum_{i=1}^{N-1}k(n)\Delta T_{i,x}^{j+1}\,\psi_{i,x}^{j}\Delta x\Delta t=-A_1-A_2 \quad (15)$$

Using the summation by parts formula to the A_2, the following expression is obtained:

$$A_2=\sum_{j=0}^{m-1}\sum_{i=1}^{N-1}\Delta T_{i,x}^{j+1}k(n)\,\psi_{i,x}^{j}\Delta x\Delta t=$$

$$=\sum_{j=0}^{m-1}\left(\Delta T_N^{j+1}k(n)\psi_{N,\bar{x}}^{j}-\Delta T_0^{j+1}k(n)\psi_{1,\bar{x}}^{j}\right)\Delta t-\sum_{j=0}^{m-1}\sum_{i=1}^{N-1}\Delta T_i^{j+1}\left(k(n)\psi_{i,x}^{j}\right)_{\bar{x}}\Delta x\Delta t$$

Assume that homogeneous boundary conditions are applied on the left boundary of the domain.

$$\psi_{1,\bar{x}}^{j}=0, j=m-1,m-2,\dots,0.$$

From equation (13), the following formula is obtained:

$$-\sum_{i=1}^{N-1}\sum_{j=0}^{m-1}\Delta T_i^{j+1}\,\psi_{i,\bar{t}}^{j+1}\Delta t\Delta x=\sum_{j=0}^{m-1}\sum_{i=1}^{N-1}\Delta T_i^{j+1}\left(k(n)\psi_{i,x}^{j}\right)_{\bar{x}}\Delta x\Delta t-\sum_{j=0}^{m-1}\Delta T_N^{j+1}k\,(n)\psi_{N,\bar{x}}^{j}\Delta t-A_1$$

After collecting similar terms, the following expression is derived:

$$-\sum_{i=1}^{N-1}\sum_{j=0}^{m-1}\Delta T_i^{j+1}\left[\psi_{i,\bar{t}}^{j+1}+k(n)\psi_{i,x\bar{x}}^{j}\right]\Delta t\Delta x=-\sum_{j=0}^{m-1}\Delta T_N^{j+1}\left[k(n)\psi_{N,\bar{x}}^{j}\right]\Delta t-A_1 \quad (16)$$

For iterations n and $n+1$, the following functionals are obtained:

$$I[n]=\sum_{j=0}^{m-1}\left(T_N^{j+1}(n)-T_{exp}^{j+1}\right)^2\Delta t\equiv I_n$$

$$I[n+1]=$$

$$=\sum_{j=0}^{m-1}\left(T_N^{j+1}(n+1)-T_{exp}^{j+1}\right)^2\Delta t\equiv I_{n+1}$$

Using the obvious formula:

$$a^2-b^2=2(a-b)b+(a-b)^2$$

the following expression is obtained

$$I_{n+1}-I_n=2\sum_{j=0}^{m-1}\Delta T_N^{j+1}\left(T_N^{j+1}(n)-T_{exp}^{j+1}\right)\Delta t+\sum_{j=0}^{m-1}\left(\Delta T_N^{j+1}\right)^2\Delta t \quad (17)$$

Based on equations (14) and (15), the adjoint problem is formulated:

$$\psi_{i,\bar{t}}^{j+1}+k(n)\psi_{i,x\bar{x}}^{j}=0 \quad (18)$$
$$i=1,2,\dots,N-1$$
$$j=m-1,m-2,\dots,0$$

At the final time $t_m = m\Delta t = T$, the following condition is imposed:

$$\psi_i^m = 0, i = 0, 1, \dots, N \quad (19)$$

At the boundary $x = 0$, Neumann conditions is imposed:

$$\psi_{1,\bar{x}}^j = 0, j = m - 1, m - 2, \dots, 0 \quad (20)$$

At the right boundary, i.e., at $x = L$, the following condition is imposed:

$$k(n)\psi_{N,\bar{x}} = 2\left(T_{\mathrm{N}}^{j+1}(n) - T_{exp}^{j+1}\right) \quad (21)$$

The systems (1)–(3) and (18)–(20) are numerically implemented using the Thomas algorithm.

After deriving the adjoint problem from equations (16) and (17), the following formula remains:

$$I_{n+1} - I_n = -A_1 + \sum_{j=0}^{m-1} \left(\Delta T_N^{j+1}\right)^2 \Delta t \quad (22)$$

Here

$$A_1 = \sum_{j=0}^{m-1} \sum_{i=1}^{N-1} \Delta k T_{i,x}^{j+1}(n+1)\psi_{i,x}^j \Delta x \Delta t$$

However

$$T_{i,x}^{j+1}(n+1) = T_{i,x}^{j+1}(n) + \Delta T_{i,x}^{j+1}$$

Thus equation (20) is written as follows:

$$I_{n+1} - I_n = \\ = -\sum_{j=0}^{m-1} \sum_{i=1}^{N-1} \Delta k\, T_{i,x}^{j+1}(n)\psi_{i,x}^j \Delta x \Delta t + R \quad (23)$$

Where $R -$ small second-order term which is determined by the following formula:

The value of Δk is selected such that the following inequality holds:

$$I_{n+1} - I_n < 0$$

Then

$$\Delta k = \sum_{j=0}^{m-1} \sum_{i=1}^{N-1} T_{i,x}^{j+1}(n)\psi_{i,x}^j \Delta x \Delta t$$

Subsequently, at each iteration, the value of the thermal conductivity coefficient is updated by minimizing the functional using the gradient descent method, as follows [12]:

$$k(n+1) = k(n) + \alpha(n)\Delta k(n)$$

where $\Delta k(n)$ represents the gradient of the functional with respect to k at iteration n, and $\alpha(n)$ is the step size that controls the magnitude of the update.

Here

$$\alpha(n) = \frac{\alpha_0}{(1+n)^\beta} \quad (24)$$

α_0, β – gradient descent parameters, $n -$ iteration number. $0 < \alpha_0, \beta < 1$

This iterative approach adjusts k in the direction of the steepest descent, ensuring convergence toward the optimal value.

Algorithm for solving the inverse problem

Step 1. Initial approximations $k(n), \alpha_0, \beta$ are specified [13].

Step 2. The direct finite-difference problem (1) – (3) is solved in the domain ω.

Step 3. The adjoint finite-difference problem (18) – (21) is solved in the domain ω.

Step 4. The value of the functional is computed.

$$I_{n+1} = \sum_{j=0}^{m-1} \left(T_N^{j+1} - T_{exp}^{j+1}\right)^2 \Delta t$$

Step 5. The value of $\Delta k(n)$ is computed as:

$$\Delta k(n) = \sum_{j=0}^{m-1} \sum_{i=1}^{N-1} T_{i,x}^{j+1}\psi_{i,x}^j \Delta x \Delta t$$

Step 6. The parameter $\alpha(n)$ is updated as $\alpha(n) = \frac{\alpha_0}{(1+n)^\beta}$, and the next approximation of the coefficient k is computed as:

$$k(n+1) = k(n) + \alpha(n)\Delta k(n)$$

Step 7. It is checked whether one of the following inequalities is satisfied:

$$|k(n+1) - k(n)| < \varepsilon_1 \text{ or } I < \varepsilon_2,$$

where $\varepsilon_1 = 10^{-5}$, $\varepsilon_2 = 10^{-6}$.

The first condition ensures that the problem has stabilized, and the change in the parameter k between iterations is negligible. The second condition ensures that the difference between the experimental and numerical values has become insignificant, confirming that the exact parameter k has been found. Small values of ε ensure the accuracy of the solution.

Step 8. If one of the inequalities is satisfied, the true value of k is found. If neither inequality is satisfied, set $n = n + 1$ and return to Step 2.

4. Results and Discussion

The Figure 1 presents the results of solving the inverse problem using the Thomas algorithm. Six cases were considered, where the initial estimate of the thermal conductivity coefficient k deviated by ±10%, ±25%, and ±50% from its exact value. Additionally, the influence of the descent parameter β in the formula (24) was investigated. Three different values of the parameter β were tested: $0.1, 0.25, 0.5$.

In all the graphs, it can be observed that the convergence of all solutions gradually approaches the exact value $k = 0.65$, regardless of the initial deviation.

It was observed, that the speed of the solution depends on the initial deviation: for negative deviations from the exact values of k, the convergence rate is practically independent of the deviation value, requiring about 160 – 210 iterations. However, for positive deviations, the convergence time increases proportionally to the deviation value, varying from 187 to 510 iterations.

Analysis of various descent parameters β showed that the fastest convergence is achieved at $\beta = 0.25$. Remarkably, even with significant initial deviations, such as +50% and –50%, the algorithm remains stable and returns the correct value of k. This emphasizes the robustness of the method under various initial assumptions.

5. Conclusion

In this paper, the inverse problem for determining the thermal conductivity coefficient k was solved using an iterative approach that included the following three main steps: a forward problem, an adjoint problem, and a gradient-based update scheme. The forward and adjoint problems were discretized using the finite difference method and solved by the Thomas algorithm. At each iteration, the discrepancy between the numerical solution and the temperature measurements was minimized to find k.

According to the obtained results, the proposed method effectively finds the thermal conductivity coefficient close to the exact value ($k = 0.65$) regardless of the initial deviation. At the same time, when setting negative initial deviations from the true value, equal to -10%, -25% and -50%, the convergence rate practically did not change and remained relatively constant. When setting positive initial deviations equal to +10%, +25% and +50%, with an increase in the initial deviations, the number of iterations increased.

The results showed that the convergence rate is sensitive to the descent parameter β, where at $\beta = 0.25$, the optimal convergence rate was obtained. One of the key numerical results obtained by the proposed model is that the algorithm demonstrated reliability and stability even in cases with large initial deviations (±50%), returning the exact values of k.

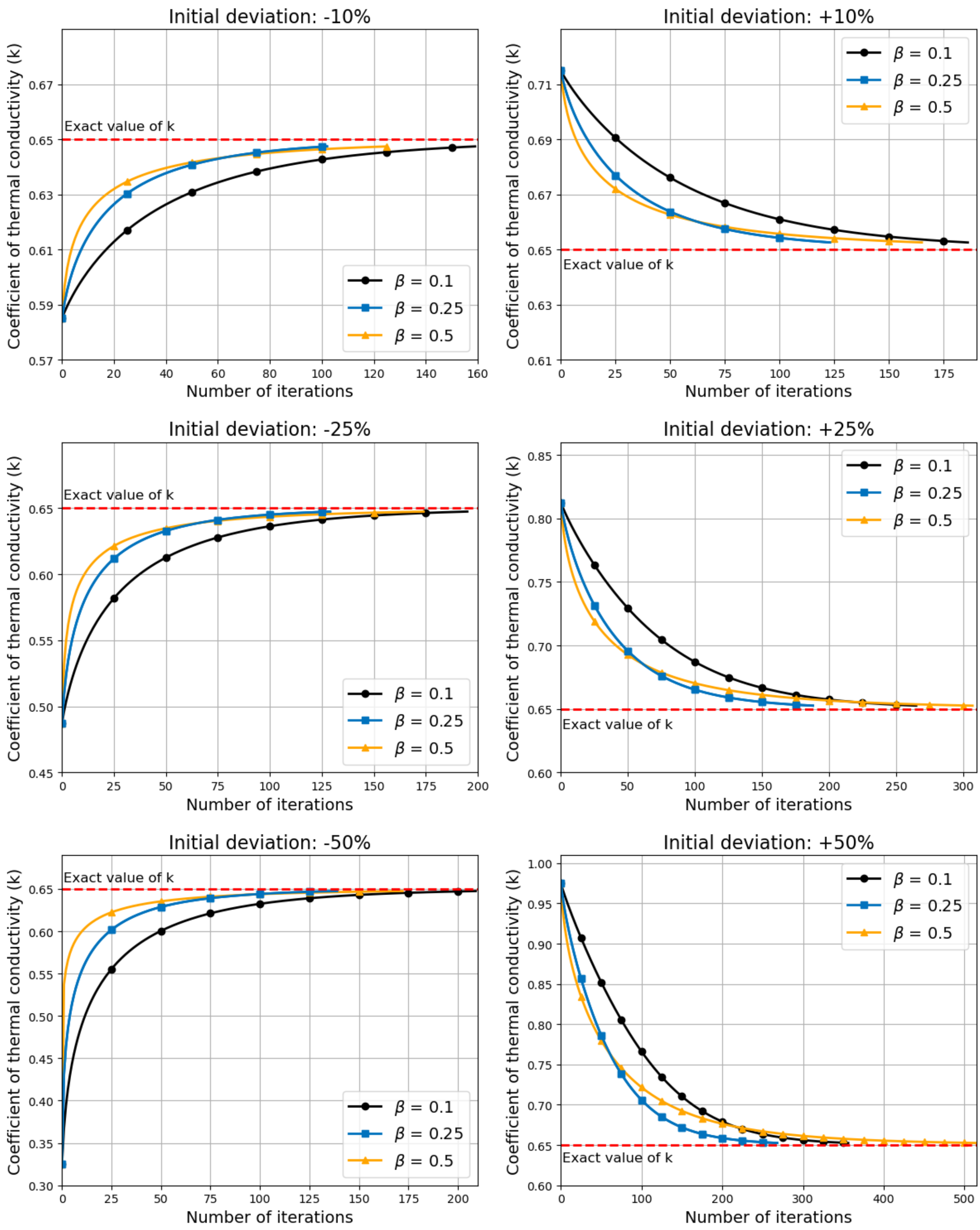

Figure 1 – Dependence of the rate of convergence of the thermal conductivity coefficient for different initial deviations from the exact value and descent parameters β

The results show that the iterative approach (using the direct problem, adjoint problem, and gradient descent) reliably converges to an exact estimate of k, even with varying initial guesses. This suggests that, under the tested scenarios and assumptions, k can be uniquely identified in practice. Additionally, exploring the sensitivity of k to noise in the data and improving the accuracy of model assumptions are promising directions for future research. These methods would further aid in studying the uniqueness of k and will be investigated in subsequent work.

The proposed method has proven to be effective for solving inverse problems of finding thermal conductivity coefficients. Due to its iterative approach, combined with the stability of the Thomas algorithm, makes it a valuable tool for practical applications in engineering and materials science, where precise determination of thermal properties is critical. Future work could explore its application to more complex multi-dimensional problems, further establishing its versatility and utility.

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Information about authors:
Aiymzhan Baitureyeva – PhD student, Al-Farabi Kazakh National University, Almaty, Kazakhstan, email: baitureyeva.aiymzhan@gmail.com
Bolatbek Rysbaiuly – Doctor of science, Professor, Astana IT University, Astana, Kazakhstan, e-mail: rysbaiuly.b@gmail.com

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