Analytical Sensitivity Analysis for 1D Thermal Diffusion Model

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Abstract

Analytical sensitivity analysis for one-dimensional (1D) thermal diffusion models provides a powerful approach to understanding how changes in input parameters affect system behavior. This study focuses on local sensitivity analysis, investigating the cooling rates of spatter deposits modeled using a 1D thermal diffusion equation. By examining small perturbations in thermal diffusivity, the analysis establishes direct relationships between material properties and cooling rates. These findings offer insights into environmental factors affecting thermal processes, contribute to the optimization of thermal management in engineering applications, and improve predictive modeling in material science.

1 Introduction

Understanding the sensitivity of mathematical models is crucial in many fields of science and engineering. A great number of studies have been conducted to predict the cooling rates of spatter deposits to better understand how these systems work. For example, previous work by Claire Elizabeth and Sergey Lapin (2021) [1] has focused on identifying the influence of changing material properties (specifically the size of clasts for a volcanic process) on the cooling time of spatter piles.

In one of the simpler cases of their work (Model 1), predicting the cooling condition of spatter deposits is one-dimensional and includes a single clast with variable material properties cooling by conduction. In her study, Claire explored heat transfer in the system using numerical methods such as finite difference and finite element methods.

For the model (Fig. 1A, B, p.18), the ground is assumed to be basalt with an initial temperature of 293 K. The clast is also basalt but has an initial temperature of either 1073 K or 1373 K. The initial temperature of the air is 293 K. This setup implies that the initial function $f(x)$ is a step function. Neumann boundary conditions (prescribed heat flux) are incorporated at the ground/air, ground/clast, clast/clast, and clast/air boundaries, while Dirichlet boundary conditions (fixed temperature) are applied along the exterior boundaries of the system. General schematics of the models can be found in Figures 1 and 2 (p.17).

This problem can then be modeled as the 1D heat diffusion equation as follows (derivation reference: MIT's PDE Class):

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}, \quad 0 < x < L,\ t > 0 \tag{1}$$

$$\text{IC: } T(x,0) = f(x),\ 0 < x < L, \tag{2}$$

$$\text{BC: } T(0,t) = T(L,t) = 0,\ t > 0. \tag{3}$$

Here, $T(x,t)$ is the temperature at point x of the object at time t, where t is time, x is the spatial dimension, and κ is the thermal diffusivity.

We will be studying this 1D case of the heat equation. In particular, we analyze how small changes in parameters affect the outcomes of partial differential equations (PDEs) can provide valuable insights. This paper focuses on sensitivity analysis of the heat equation, a fundamental PDE used to model thermal diffusion. Such analysis is relevant in applications ranging from material science to environmental studies.

The problem addressed in this paper is the derivation and analysis of the sensitivity of the temperature distribution to changes in the thermal diffusivity parameter κ. By understanding this sensitivity, we can better comprehend how variations in material properties or environmental factors influence thermal processes.

This study is motivated by the need for precise modeling and robust predictions in systems where thermal diffusivity varies due to external factors or material heterogeneity. For instance, understanding these effects can improve the design of heat-resistant materials or optimize thermal management systems in engineering applications.

The scope of this work is outlined as follows: In the next section, we provide background material on sensitivity analysis and the heat equation. Following this, we derive the sensitivity equations and discuss their solutions. Here, in this project, we aim to study this case analytically as much as possible, make comparisons with numerical solutions of the work by Claire Elizabeth [1], and analyze specific examples to illustrate the impact of parameter changes. Finally, we conclude with a summary of findings and reflections on the broader implications of this study.

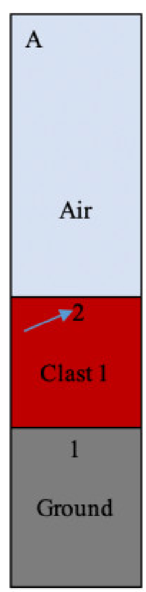

Figure 1A-B. (A) Schematic of one-dimensional thermal diffusion single clast model of a hot clast (red) emplaced on to the ground (gray) surrounded by air (blue). For Model 1, boundaries 1 and 2 incorporate heat transfer by conduction.

Figure 1: Explanation of the origin of the model

2 Analytical Sensitivity Analysis for 1D Thermal Diffusion Model at a Particular Point

Here, in this main body paragraph, using a change of variables, we get rid of the κ to have an even simpler version of the given PDE. Then we use the solution of this attained simple (monic) PDE to obtain the solution of the (non-monic) PDE with κ given in (1). Using this solution depending on κ, we can take the (ordinary) derivative to determine how a small change in κ influences the solution $T(x,t)$ at a specified point x_0, t_0, or specifically, what changes in κ cause the highest sensitivity of the temperature at that point (x_0, t_0). To verify our results in this paragraph, we try to make comparisons with the numerical work by Elizabeth Claire [1].

2.1 Solving the given model equation in (1)-(3):

Start with the fundamental equations of the given model (1)-(3):

$$\frac{1}{\kappa} \cdot \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} \tag{4}$$

Consider the following change of variables:

$$\tau = \kappa \cdot t \tag{5}$$

Then,

$$\frac{\partial T}{\partial t} = \kappa \cdot \frac{\partial T}{\partial \tau}, \tag{6}$$

$$\frac{\partial^2 T}{\partial x^2} = \frac{\partial^2 T}{\partial x^2} \tag{7}$$

$$u(x,0) = f(x), \quad 0 < x < L, \tag{8}$$

$$u(0,\tau) = u(L,\tau) = 0, \quad \tau > 0 \tag{9}$$

and the given heat equation (1)-(3) becomes

$$\frac{\partial T}{\partial \tau} = \frac{\partial^2 T}{\partial x^2}, \quad 0 < x < L,\ \tau > 0 \tag{10}$$

$$\text{IC: } T(x,0) = f(x),\ 0 < x < L, \tag{11}$$

$$\text{BC: } T(0,\tau) = T(L,\tau) = 0,\ \tau > 0. \tag{12}$$

for which we know the solution of the form (a PDE textbook by E.C. Zachmonoglou and Dale W. Thoe [2]):

$$T(x,\tau) = \sum_{n=1}^{\infty} C_n \cdot \sin\left(\frac{(2n-1)\pi x}{2L}\right) e^{-\frac{(2n-1)^2\pi^2}{4L^2}\tau} \tag{13}$$

where C_n is the Fourier sine series of the function f(x), and as follows:

$$C_n = \frac{2}{L}\int_0^L f(x)\sin\left(\frac{n\pi x}{L}\right)\, dx \tag{14}$$

Now replacing back the τ in this solution (13) by $\kappa\cdot$ t based on (5), we get the solution for the given (1)-(3) equation as follows:

$$T(x,t) = \sum_{n=1}^{\infty} C_n \cdot \sin\left(\frac{(2n-1)\pi x}{2L}\right) e^{-\frac{(2n-1)^2\pi^2}{4L^2}\kappa t} \tag{15}$$

is a solution for the given heat equation (1)-(3). Here T is the temperature solution, t is time, x is the spatial dimension, and κ is the thermal diffusivity.

2.2 Perturbation of Parameters:

Consider small perturbations in a parameter (e.g., thermal diffusivity κ). Let $\kappa = \kappa_0 + \delta$, where δ is a small change. The solution to the heat equation can then be expressed in terms of this perturbed parameter.

2.3 Derive the Sensitivity of the Solution $T(x,t)$ Function:

In this step, we analyze the sensitivity of the temperature $T(x,t)$ locally, at a specified point (x_0, t_0). That is, we want to know how much the change in κ (small perturbation δ in step 2) affects the point x_0 at time t_0. With a little bit of abuse of mathematical notation, the solution function $T(x,t)$ in (15) can then be written as:

$$T(x,t) = T(x,t,\kappa) = T(x_0,t_0,\kappa) = T(\kappa) \tag{16}$$

The sensitivity of the temperature $T(\kappa)$ (note $T(\kappa)$ being a function of one variable κ only) with respect to κ can be expressed as:

$$S_\kappa = S(\kappa) = \frac{dT}{d\kappa} \tag{17}$$

This derivative shows how sensitive the temperature of the point x_0 at time t_0 is to changes in the thermal diffusivity. Deriving this function involves differentiating the solution of the heat equation with respect to κ. In this paragraph, we obtain S_κ by directly differentiating the solution $T(x,t)$ with respect to κ.

2.4 Evaluate the Sensitivity:

Let us clarify the above-mentioned step. We can compute $S_\kappa = \frac{dT}{d\kappa}$ because the solution $T(x,t)$ in (13) converges absolutely uniformly (as noted in E.C. Zachmonoglou and Dale W. Thoe, §9.2). By performing this differentiation, we can evaluate how changes in κ affect the solution at specific times t_0 and locations x_0 within the defined domain. Let us calculate S_κ:

$$
\begin{aligned}
S_\kappa &= \frac{dT}{d\kappa} \\
&= \frac{d}{d\kappa}\left(\sum_{n=1}^{\infty} C_n \cdot \sin\left(\frac{(2n-1)\pi x_0}{2L}\right) e^{-\frac{(2n-1)^2\pi^2}{4L^2}\kappa t_0}\right) \\
&= \sum_{n=1}^{\infty} C_n \cdot \sin\left(\frac{(2n-1)\pi x_0}{2L}\right) \frac{d}{d\kappa}\left(e^{-\frac{(2n-1)^2\pi^2}{4L^2}\kappa t_0}\right) \\
&= \sum_{n=1}^{\infty} C_n \cdot \sin\left(\frac{(2n-1)\pi x_0}{2L}\right) \cdot e^{-\frac{(2n-1)^2\pi^2}{4L^2}\kappa t_0} \cdot \left(-\frac{(2n-1)^2\pi^2}{4L^2} t_0\right).
\end{aligned} \tag{18}
$$

Since the point (x_0, t_0) is chosen arbitrarily, these concepts hold for all points in the domain. Thus, the sensitivity of the temperature function T can be expressed as:

$$
S_\kappa = \sum_{n=1}^{\infty} C_n \cdot \sin\left(\frac{(2n-1)\pi x_0}{2L}\right) \cdot e^{-\frac{(2n-1)^2\pi^2}{4L^2}\kappa t_0} \cdot \left(-\frac{(2n-1)^2\pi^2}{4L^2} t_0\right). \tag{19}
$$

By using Equation (17) to solve for dT, we obtain:

$$
\begin{aligned}
dT &= S_\kappa \cdot d\kappa \\
&= \left(\sum_{n=1}^{\infty} C_n \cdot \sin\left(\frac{(2n-1)\pi x_0}{2L}\right) \cdot e^{-\frac{(2n-1)^2\pi^2}{4L^2}\kappa t_0} \cdot \left(-\frac{(2n-1)^2\pi^2}{4L^2} t_0\right)\right) \cdot d\kappa.
\end{aligned} \tag{20}
$$

The general result of this evaluation is the change in temperature, dT:

$$
dT = \left(\sum_{n=1}^{\infty} C_n \cdot \sin\left(\frac{(2n-1)\pi x_0}{2L}\right) \cdot e^{-\frac{(2n-1)^2\pi^2}{4L^2}\kappa t_0} \cdot \left(-\frac{(2n-1)^2\pi^2}{4L^2} t_0\right)\right) \cdot d\kappa. \tag{21}
$$

Equation (21) represents the general temperature sensitivity for changes in κ. If we denote $d\kappa = \delta$ (a small perturbation), the equation becomes:

$$
dT = \left(\sum_{n=1}^{\infty} C_n \cdot \sin\left(\frac{(2n-1)\pi x_0}{2L}\right) \cdot e^{-\frac{(2n-1)^2\pi^2}{4L^2}(\kappa_0+\delta) t_0} \cdot \left(-\frac{(2n-1)^2\pi^2}{4L^2} t_0\right)\right) \cdot \delta. \tag{22}
$$

Here, κ_0 represents the initial thermal diffusivity, and δ is a small perturbation applied to this diffusivity. This expression enables us to analyze how changes in κ influence the temperature at specified points in the domain.

2.5 Interpretation of Results:

We have two main results to discuss in this paragraph:

First, by analyzing S_κ in (19), we can observe high values of $|S_\kappa|$ indicate high sensitivity, meaning that exactly what changes in κ can lead to the greatest or least changes in temperature. Note that, with the introduction of step 4, S_κ is continuous because the temperature $T(x,t)$ is continuous. Since $T(x,t)$ is a sum of absolutely uniformly convergent series, its derivative, S_κ, must also be continuous. For a closed domain, we can consider the closure of the domain (x,t), and therefore, the Extreme Value Theorem (EVT) can be applied.

Second, for positive perturbations, $0 < \delta_1 < \delta_2$ in κ, the corresponding temperature changes dT with exponential terms are as follows:

$$0 < \delta_1 < \delta_2, \tag{23}$$

$$e^{-\frac{(2n-1)^2\pi^2}{4L^2}(\kappa_0+\delta_1)t_0} > e^{-\frac{(2n-1)^2\pi^2}{4L^2}(\kappa_0+\delta_2)t_0}, \tag{24}$$

$$|dT_1| > |dT_2|. \tag{25}$$

We find that $|dT_1| > |dT_2|$ because the C_n and sine terms are the same in both cases, but their signs may differ. The absolute values of dT_1 and dT_2 provide a true relationship between the two, regardless of whether the C_n and sine terms are positive or negative. From equations (23) and (25), it follows that **as thermal diffusivity increases, the change in temperature decreases**.

To further explain, consider a small time interval $(t_0, t_0 + dt)$ around time t_0. The rate of change of temperature, $\frac{dT}{dt}$,

We observe that $|dT_1| > |dT_2|$ because the C_n and sine terms are the same for both cases, but their signs may differ. The absolute value relationship ensures that $|dT_1| > |dT_2|$ holds true, regardless of whether the C_n and sine terms are negative or positive. From equations (23) and (25), it follows that **as thermal diffusivity**

increases, the change in temperature decreases.

Moreover, in the considered small time interval $(t_0, t_0 + dt)$, the **rate of change in temperature, $\frac{dT}{dt}$, decreases as thermal diffusivity increases**, as shown by equation (25):

$$0 < \delta_1 < \delta_2, \tag{26}$$

$$|dT_1| > |dT_2|, \tag{27}$$

$$\frac{|dT_1|}{dt} > \frac{|dT_2|}{dt}. \tag{28}$$

This result is consistent with the numerical studies by Claire Elizabeth [1], which state:

> *"Model 1 is a one-dimensional thermal diffusion model for a single clast that incorporates heat transfer by conduction. This model is set up such that the material properties change between the clast and the air, and heat is transferred across this boundary through conduction. Given this framework, we tested clast size, amount of vesicularity, and initial temperature. The results of Model 1 indicate that increasing clast size yields a greater time to cool to the glass transition temperature (Figure 3A).* ***As clast size increases(which in turn causes thermal diffusivity*** *$[mm^2/sec]$* ***to increase by Wikipedia[7], the cooling rate decreases (Figure 3B).*** *Clasts with high initial temperatures will take longer to cool to the glass transition temperature than those with lower initial temperatures (Figure 3A). However, neither initial temperature nor vesicularity impacts cooling rates except for the scenarios with small clast sizes (Figure 3B, Page 13)."*

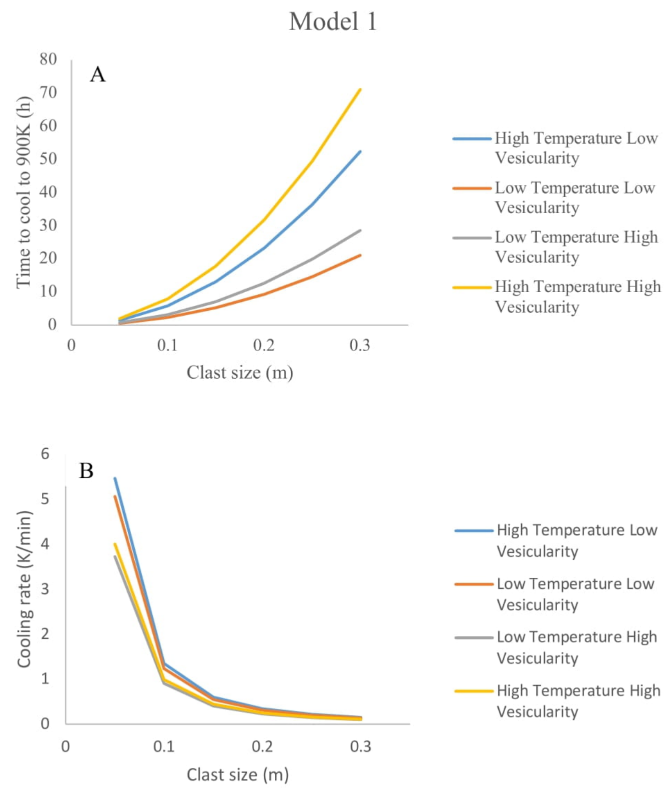

Figure 3A-B. (A) One-dimensional conduction thermal diffusion model results showing clast size (m) vs. time to cool to 900K (hours). (B) One-dimensional conduction thermal diffusion model results showing clast size (m) vs. cooling rate (K/min). A high initial temperature of 1373 K is used and a low initial temperature of 1073 K is used.

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Figure 2: Numerical solutions of this model by Claire Elizabeth [1].

3 Analytical Sensitivity Analysis for the 1D Thermal Diffusion Model in the Entire Domain

To begin, recall from the previous section that we initially focused on a particular point, essentially fixing a point, and allowed κ to change infinitesimally in order to study how this change influences the temperature at that specific point. This represents a local sensitivity analysis. In contrast, this section is dedicated to studying how a change in κ, denoted as $\partial\kappa$, affects the solution $T(x,t)$ over the **entire domain** (x,t). In other words, we now consider the variation of κ and analyze its influence on the temperature at any point (x,t) in the domain. This is a slight generalization (and a different perspective) compared to the approach in the previous section. This section outlines the derivation of a sensitivity equation for the one-dimensional heat equation with respect to the thermal diffusivity parameter κ.

3.1 Derivation of the Sensitivity Function

The original partial differential equation governing the temperature distribution is given by equations (1)-(3):

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}, \quad 0 < x < L,\ t > 0,$$

$$\text{IC: } T(x,0) = f(x),\ 0 < x < L,$$

$$\text{BC: } T(0,t) = T(L,t) = 0,\ t > 0.$$

where T is the temperature, t is time, x is the spatial coordinate, and κ is the thermal diffusivity.

The sensitivity function $S_\kappa(x,t)$ is defined as the partial derivative of the temperature with respect to κ:

$$S_\kappa(x,t) = \frac{\partial T}{\partial \kappa}, \tag{29}$$

which quantifies how sensitive the temperature profile is to a change $\partial\kappa$ in the thermal diffusivity.

3.2 Differentiating the Heat Equation

Differentiating both sides of the heat equation with respect to κ, we obtain:

$$\frac{\partial}{\partial\kappa}\left(\frac{\partial T}{\partial t}\right) = \frac{\partial}{\partial\kappa}\left(\kappa\frac{\partial^2 T}{\partial x^2}\right). \tag{30}$$

This partial differentiation requires the application of the chain rule and other differentiation techniques to handle the terms involving κ.

3.3 Calculate the Partial Derivatives

First, note that $T(x,t)$ is a sufficiently continuous function (as concluded in main body paragraph 1), and its mixed partial derivatives commute. Therefore, applying this to the LHS of the equation in (30), we obtain:

$$\text{LHS} = \frac{\partial}{\partial\kappa}\left(\frac{\partial T}{\partial t}\right) = \frac{\partial}{\partial t}\left(\frac{\partial T}{\partial\kappa}\right) \tag{31}$$

Next, applying the product rule and the chain rule to the differentiation on the RHS of the equation in (30), we get:

$$\text{RHS} = \frac{\partial^2 T}{\partial x^2} + \kappa\frac{\partial}{\partial\kappa}\left(\frac{\partial^2 T}{\partial x^2}\right) \tag{32}$$

Now, using $\frac{\partial T}{\partial\kappa} = S_\kappa$ for the LHS expression in (31), we can rewrite it as:

$$\text{LHS} = \frac{\partial}{\partial t}\left(\frac{\partial T}{\partial\kappa}\right) = \frac{\partial S_\kappa}{\partial t} \tag{33}$$

For the RHS expression in (32), we know the fact that $\frac{\partial^2 T}{\partial x^2} = \frac{1}{\kappa}\frac{\partial T}{\partial t}$, as given by the heat equation (1). Assuming the commutative property of mixed partials of $T(x,t)$ with respect to κ, and applying $\frac{\partial T}{\partial\kappa} = S_\kappa$ again, we can simplify the RHS expression as follows:

$$\begin{aligned}
\text{RHS} &= \frac{\partial^2 T}{\partial x^2} + \kappa \frac{\partial}{\partial \kappa}\left(\frac{\partial^2 T}{\partial x^2}\right) \\
&= \frac{1}{\kappa}\frac{\partial T}{\partial t} + \kappa \frac{\partial^2}{\partial x^2}\left(\frac{\partial T}{\partial \kappa}\right) \\
&= \frac{1}{\kappa}\frac{\partial T}{\partial t} + \kappa \frac{\partial^2 S_\kappa}{\partial x^2}
\end{aligned}$$

Hence, the RHS becomes:

$$\text{RHS} = \frac{1}{\kappa}\frac{\partial T}{\partial t} + \kappa \frac{\partial^2 S_\kappa}{\partial x^2} \tag{34}$$

Finally, by setting the LHS equal to the RHS, we get:

$$\begin{aligned}
&\text{LHS} = \text{RHS} \\
&\frac{\partial S_\kappa}{\partial t} = \frac{1}{\kappa}\frac{\partial T}{\partial t} + \kappa \frac{\partial^2 S_\kappa}{\partial x^2}
\end{aligned} \tag{35}$$

Substituting $\frac{\partial T}{\partial t}$ from the original heat equation (1), we obtain:

$$\frac{\partial S_\kappa}{\partial t} = \frac{\partial^2 T}{\partial x^2} + \kappa \frac{\partial^2 S_\kappa}{\partial x^2} \tag{36}$$

With some further algebra and by substituting the initial and boundary conditions from equations (2)-(3) into the sensitivity function $S_\kappa(x, t)$, we can derive a PDE that will be presented in the next step. Note that our boundary conditions are Dirichlet, which were chosen for computational simplicity. However, any initial and boundary conditions could work, following similar steps, as long as the given governing PDE is well-posed.

$$\text{IC: } S_\kappa(x, 0) = \frac{\partial T(x, 0)}{\partial \kappa} = \frac{\partial f(x)}{\partial \kappa},\ 0 < x < L,$$

$$\text{BC: } S_\kappa(0,t) = \frac{\partial T(0,t)}{\partial \kappa} = \frac{\partial 0}{\partial \kappa} = 0,\ t > 0$$
$$\text{BC: } S_\kappa(L,t) = \frac{\partial T(L,t)}{\partial \kappa} = \frac{\partial 0}{\partial \kappa} = 0,\ t > 0$$

3.4 Final Sensitivity Equation

This leads us to the final sensitivity partial differential equation (PDE):

$$\frac{\partial S_\kappa}{\partial t} = \kappa \frac{\partial^2 S_\kappa}{\partial x^2} \tag{37}$$

The corresponding initial and boundary conditions are:

$$\text{IC: } S_\kappa(x,0) = \frac{\partial f(x)}{\partial \kappa},\ 0 < x < L \tag{38}$$

$$\text{BC: } S_\kappa(0,t) = S_\kappa(L,t) = 0,\ t > 0. \tag{39}$$

This equation indicates that the sensitivity function $S_\kappa(x,t)$ evolves according to a diffusion process modulated by the thermal diffusivity κ. We can solve this PDE (37)-(39) either analytically or numerically to evaluate how changes in κ affect the solution at any time t and at locations x in the domain.

For example, similar to Elizabeth Claire's Model 1 [1], suppose the initial condition $f(x)$ is a step function for the temperature, defined as:

$$T(x,0) = T_0 \quad \text{for} \quad x \leq 0, \quad T(x,0) = 0 \quad \text{for} \quad x > 0,$$

with κ being the parameter of interest. While the analytical solution and its sensitivity might appear complex, they are derived from the solutions to the heat equations (1)-(3) and (37)-(39), respectively, following the method outlined above.

3.5 Interpret the Results

The analytical derivation provides a clear mathematical framework for understanding how variations in thermal diffusivity affect the temperature at any point (x, t) in the domain within a one-dimensional thermal diffusion setting. This sensitivity PDE (37)-(39) can be solved in conjunction with the original heat equation (1)-(3) to gain a deeper insight into the impacts of the parameter κ.

4 Conclusion

Throughout this paper, we have locally analyzed the sensitivity of the solution to the given partial differential equation (PDE). Other types of local analysis can follow similar steps. In contrast to global sensitivity, where perturbations can affect multiple variables simultaneously, this paper focused on the use of ordinary and partial derivatives to explore local sensitivity. However, there was a need to employ matrices, and certain statistical methods, particularly in Main Body 2, where we dealt with the sensitivity function of three variables $S_\kappa(x, t) = S(\kappa, x, t)$ (a paper by Viktoria Savatorova [6]). We attempted to avoid unnecessary complexities, and instead, we first allowed κ to vary by a specific amount $\partial\kappa$, keeping it fixed afterward. This approach led us to derive the diffusion PDE (37)-(39) for the sensitivity function $S_\kappa(x, t)$. Naturally, this process comes with both advantages and limitations, which are outlined below:

Advantages:

- Provides exact relationships between parameters and outputs.
- Helps in understanding the direct impact of each parameter under controlled perturbations.
- Useful for validating numerical models and conducting theoretical studies.

Limitations:

- Only feasible for models that can be solved analytically.
- Often requires simplifications that may not be applicable in all practical scenarios.

- Can be mathematically intensive and may require advanced mathematical tools.

In conclusion, analytical sensitivity analysis in cases like the thermal diffusion model is a powerful approach, but it is highly dependent on the ability to solve the model equations explicitly. For more complex systems or models involving non-linear behavior, numerical methods—or a combination of analytical and numerical methods—may be necessary.

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