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以數值方法估計熱傳導反問題的解
Numerical Estimation for Inverse Heat Conduction Problems

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# 國立臺灣大學碩士學位論文口試委員會審定書 

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Numerical Estimation for Inverse Heat Conduction Problems

本論文係張繁可君（R05246010）在國立臺灣大學應用數學科學研究所完成之碩士學位論文，於民國109年1月17日承下列考試委員審查通過及口試及格，特此證明。

口試委員：

$\qquad$

系主任，所長 $\qquad$

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## 摘要

反問題是從測量的結果反推回起始原因，而熱傳導方程是描述熱量藉由傳導方式傳遞能量的過程，本篇探討的問題分爲兩種，從某個特定位置的邊界條件反推回原點位置的邊界條件，以及從某個時間點的温度分佈反推回初始條件。爲了方便研究，先給定起始原因，找到某個時間的結果，主要目標就是從此結果反推回起始原因，得到的解可以和眞正的起始原因作比較。

使用數値方法將熱傳導方程的解析解離散化，得到的線性系統是非適定性問題，由截斷奇異值分解方法可將其正規化，進行逆運算之後會得到解，若起始原因的狀態具有足夠的平滑性，則這個解的趨勢和眞正的起始原因會很接近。

關鍵字：反／逆問題，熱傳導方程，數値方法，離散化，截斷奇異値分解，正規化

## Abstract

Inverse problems recover the causes from the effects. And heat conduction equations describe the process of energy transfer by heat conduction. In this thesis, we focus on calculating the boundary condition at the origin from the other boundary condition and recovering the initial condition from the temperature distribution at a certain time. For the convenience of research, the causes are given at first and the effects are found directly. The goal is to recover the causes from the effects. The results can be compared with the real causes.

The analytical solutions of the heat conduction equations are discretized with some numerical methods. Then, the linear system obtained is an ill-posed problem. It can be regularized by the truncated singular value decomposition. If the state of the causes is smooth enough, the trend of the solution of the regularized problem with inverse operation is approaching to the real causes.

Keywords: Inverse Problems, Heat Conduction Equations, Numerical Methods, Discretization, Truncated Singular Value Decomposition, Regularization

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## Chapter 1

## Introduction

In this chapter, general inverse problems and thesis topics are introduced.

### 1.1 Inverse problems

An inverse problem is the inverse of a forward (direct) problem. A forward problem is to find the effects from the causes, and an inverse problem one starts with the effects and then calculates the causes [6]. There are several different kinds of inverse problems. In image processing, for example, the forward problem is to find the result if there is some noise of the original picture. The inverse problem is to recover the sharp image from a given blurry image and it is known as deblurring. The sample example is shown in Fig. 1.1. The forward problem is from (a) to (b) and the inverse problem is the opposite direction.


Figure 1.1: Sample example in image processing.

The general model of the forward problem is constructed as follows:

$$
\begin{equation*}
b=T(x)+\varepsilon_{m}, \tag{1.1}
\end{equation*}
$$

where $b$ is the effect, $T$ is the forward operator, $x$ is the cause and $\varepsilon_{m}$ is the error term coming from measurement noise. In the case of the example shown in Fig. 1.1, $T^{-1}$ is the deblurring operator. Furthermore, if the forward map is a linear system, then the model can be written as the linear system

$$
\begin{equation*}
b=A x+\varepsilon_{m}, \tag{1.2}
\end{equation*}
$$

where $b \in \mathbf{R}^{m}$ is the effect, $A \in \mathbf{R}^{m \times n}$ is the forward linear operator, $x \in \mathbf{R}^{n}$ is the cause, and $\varepsilon_{m} \in \mathbf{R}^{m}$ is the measurement error. Once the model has been constructed, the solution of the inverse problem is considered as

$$
\begin{equation*}
x \approx A^{-1} b . \tag{1.3}
\end{equation*}
$$

For a well-posed inverse problem, it is easy to recover the causes with the given effects. However, solving an ill-posed inverse problem is much harder. It is noticed that a well-posed problem is introduced by Jacques Hadamard [2]:
$H_{1}$ : Existence. There should be at least one solution.
$H_{2}$ : Uniqueness. There should be at most one solution.
$H_{3}$ : Stability. The solution must depend continuously on data.
If the operator is linear, this definitions are equivalent to:
$H_{1}^{*}$ : A is surjective (onto).
$H_{2}^{*}$ : A is injective (one-to-one).
$H_{3}^{*}: A^{-1}$ is continuous.
The problem is ill-posed if at least one of the conditions $H_{1}-H_{3}$ fails. If $H_{1}$ fails, then to solve this problem is non-sense. $H_{2}$ fails when the kernel of $A$ contains more than one element, that is $\operatorname{Ker}(A) \neq\{0\}$. All elements in coset $\{x+\operatorname{Ker}(A)\}$ are the solution of the inverse problem. In this case, the restriction of $A$ to $(\operatorname{Ker}(A))^{\perp}$ is considered to ensure the uniqueness, where $(\operatorname{Ker}(A))^{\perp}$ is the orthogonal complement of the subspace $\operatorname{Ker}(A)$. For the problem of finite dimension, $(\operatorname{Ker}(A))^{\perp}$ equals to $\operatorname{Range}\left(A^{*}\right)$
which is the range of the adjoint of $A$. If $H_{3}$ fails, then the inverse crime occurs and $x=A^{-1}\left(b-\varepsilon_{m}\right)=A^{-1} b-A^{-1} \varepsilon_{m}$. The term $A^{-1} \varepsilon_{m}$ may be very large even if $\varepsilon_{m}$ is very small. Thus, the results cannot be trusted. Calculating the condition number of $A$ is a way to discriminate whether the problem is well-posed or not. See A. 1 for more details.

Large condition number $\kappa(A)$ means $A$ is ill-posed. The relative error $\varepsilon\left(x^{*}\right)$ may be so large even if using the more precise computer systems. Moreover, there exists measurement errors in the system concerned. To overcome this, truncated singular value decomposition (TSVD) helps to find the more stable solution [3]. See A. 2 for more details. The reduced form of singular value decomposition is used to improve computing efficiency. In this thesis, we focus on TSVD to solve inverse heat conduction problems. The mathematical model is given in the next section.

### 1.2 Thesis topics

There are three classifications of inverse problems: determination of the initial condition of the system, determination of the boundary conditions of the system and identification of physical parameters or parameter identification of the system. In this thesis, only the initial or the boundary conditions problems of the heat conduction equations are studied. The schematic diagrams are shown in Fig. 1.2. The horizontal axis is the space $\mathbf{x}$ and the vertical axis is time $\mathbf{t}$. In Fig. 1.2 (a) which is the initial condition case, $f(x)$ is the cause and $g(x)$ is the effect. In Fig. 1.2 (b) which is the boundary condition case, $h(t)$ is the cause and $s(t)$ is the effect.


Figure 1.2: The schematic diagrams of one-dimensional problems.

To derive the heat conduction equation, it is assumed that:

1. All physical parameters including the density, the specific heat capacity and the thermal conductivity of the system are constants.
2. The temperature changes immediately when energy enters into the small volume.
3. The temperature is uniform in the small volume.

The system is chosen as a small volume region. From energy balance:

$$
\text { storage }=\text { in }- \text { out }+ \text { generation } .
$$

In the case, the generation equals to 0 . The relation can be written as

$$
\begin{equation*}
\frac{\Delta(\rho \Delta V C u)}{\Delta t}=-\oint_{S} \mathbf{J} \cdot \mathbf{n} d S, \tag{1.4}
\end{equation*}
$$

where $\Delta$ is the difference operator, $\rho$ is the density of the system, $\Delta V$ is the volume of the system which is not a function of time $t, C$ is the specific heat capacity of the system, $u$ is the temperature of the system, $\oint_{S}$ is the surface integral of a vector field over a closed surface $S$ which is the surface area of the system, $\mathbf{J}$ is heat flux, $\mathbf{n}$ is the unit normal vector of the surface area of the system and $\mathbf{J} \cdot \mathbf{n}$ is the inner product of $\mathbf{J}$ and $\mathbf{n}$. The minus symbol is because $\mathbf{n}$ is outer-pointing normal. The integration without the minus symbol equals to the energy out minus the energy in. Moreover, from Fourier's law, we have

$$
\begin{equation*}
\mathbf{J}=-D \nabla u, \tag{1.5}
\end{equation*}
$$

where $D$ is the thermal conductivity of the system, and $\nabla u$ is the gradient of the temperature. The minus symbol is due to the direction of heat flux which is from high temperature area to low temperature area. On the other hand, from divergence theorem, we have

$$
\begin{equation*}
\oint_{S} \mathbf{J} \cdot \mathbf{n} d S=\int_{V} \nabla \cdot \mathbf{J} d V \tag{1.6}
\end{equation*}
$$

where $\nabla \cdot \mathbf{J}$ is the divergence of heat flux and $\int_{V}$ is the volume integral. From the assumption 1 and $\Delta V$ is not a function of $t$, the equation (1.4) can be written as

$$
\begin{equation*}
\rho C \frac{\Delta u}{\Delta t}=-\frac{1}{\Delta V} \int_{V} \nabla \cdot(-D \nabla u) d V=\frac{D}{\Delta V} \int_{V} \nabla^{2} u d V \tag{1.7}
\end{equation*}
$$

where $\nabla^{2} u$ is the Laplacian of the temperature.

Let $\Delta V$ approach to 0 and $\Delta t$ tend to 0 , then the equation is read as

$$
\begin{equation*}
\frac{\partial u}{\partial t}=\frac{D}{\rho C} \nabla^{2} u=\beta \nabla^{2} u \tag{1.8}
\end{equation*}
$$

where $\beta=\frac{D}{\rho C}$ is the thermal diffusivity. Since $\beta$ is constant, the equation (1.8) is linear. For one-dimensional case, the equation becomes

$$
\begin{equation*}
\frac{\partial u}{\partial t}=\beta \frac{\partial^{2} u}{\partial x^{2}} \tag{1.9}
\end{equation*}
$$

Consider the domain in $x \in[0, L]$ and $t \in[0, T]$. If the temperature distribution in the domain at $t=0$ is $f(x)$, then the initial condition is

$$
\begin{equation*}
u(x, 0)=f(x) . \tag{1.10}
\end{equation*}
$$

If the temperature is constant $u_{0}$ in the left region of the domain and there is no heat loss on the right boundary, then the boundary conditions are

$$
\begin{align*}
u(0, t) & =u_{0},  \tag{1.11a}\\
\frac{\partial u}{\partial x}(L, t) & =0 . \tag{1.11b}
\end{align*}
$$

Let $\bar{u}=\frac{u-u_{0}}{u_{0}}, \bar{t}=\frac{t}{T}$ and $\bar{x}=\frac{x}{L}$, then the dimensionless equation is obtained,

$$
\begin{equation*}
\frac{\partial \bar{u}}{\partial \bar{t}}=\frac{\beta T}{L^{2}} \frac{\partial^{2} \bar{u}}{\partial \bar{x}^{2}}=\alpha \frac{\partial^{2} \bar{u}}{\partial \bar{x}^{2}}, \tag{1.12}
\end{equation*}
$$

where $\alpha=\frac{\beta T}{L^{2}}$. The initial condition is transformed to

$$
\begin{equation*}
\bar{u}(\bar{x}, 0)=\frac{f(\bar{x} L)-u_{0}}{u_{0}}=\bar{f}(\bar{x}) . \tag{1.13}
\end{equation*}
$$

And the boundary conditions are transformed to

$$
\begin{align*}
\bar{u}(0, \bar{t}) & =0,  \tag{1.14a}\\
\frac{\partial \bar{u}}{\partial \bar{x}}(1, \bar{t}) & =0 . \tag{1.14b}
\end{align*}
$$

These initial and boundary conditions appear to be more simple. In addition, it is showed that the homogeneous boundary conditions contain physical meaning. For convenience, the equation is written as

$$
\begin{equation*}
u_{t}-\alpha u_{x x}=0, \tag{1.15}
\end{equation*}
$$

where $u_{t}=\frac{\partial \bar{u}}{\partial \bar{t}}$ and $u_{x x}=\frac{\partial^{2} \bar{u}}{\partial \bar{x}^{2}}$. We use this form in the rest of this thesis.

### 1.3 Outlines

The concepts of inverse problems are in section 1.1 and thesis topics inverse heat conduction problems (IHCP) are in section 1.2. In chapter 2, the IHCP problems in semi-infinite domain are considered. The Green's functions are used to solve the forward problems and the finite difference methods are used to validate the solutions in section 2.1. The models which are constructed by the solutions from the Green's functions and the methods to solve these problems are in section 2.2. The results are shown in section 2.3. In chapter 3, the IHCP problems in finite domain are considered. Separation of variables is used to solve the forward problems in section 3.1. The solutions from this method are validated by substituted into the equations directly. The models which are constructed by the solutions from separation of variables and the methods to solve these problems are in section 3.2. The results are shown in section 3.3. The conclusions are in chapter 4 . Some supplementary materials are in appendix A including condition numbers, TSVD and the details about Green's functions, finite difference methods and separation of variables. Sample matlab codes are in appendix B.

## Chapter 2

## Heat conduction problems in

## semi-infinite domain

In this chapter, the heat conduction equation in semi-infinite domain and $\alpha=1$ is considered.

$$
\begin{equation*}
u_{t}-u_{x x}=0, \quad 0 \leq x<\infty, \quad 0 \leq t<\infty . \tag{2.1}
\end{equation*}
$$

The initial condition is assumed to be zero:

$$
\begin{equation*}
u\left(x, 0^{+}\right)=0 . \tag{2.2}
\end{equation*}
$$

Two different boundary conditions are used and they are the causes in this chapter:

1. The first kind boundary condition is

$$
\begin{equation*}
u(0, t)=h_{f}(t) . \tag{2.3}
\end{equation*}
$$

2. The second kind boundary condition is

$$
\begin{equation*}
u_{x}(0, t)=h_{s}(t) . \tag{2.4}
\end{equation*}
$$

The thermal sensor is set at $x=1$ and the temperature measured is denoted as $s(t)$ which is the effect.

$$
\begin{equation*}
u(1, t)=s(t) . \tag{2.5}
\end{equation*}
$$

The schematic diagram of the problem in this chapter is shown in Fig. 1.2 (b).

### 2.1 Methods for forward problems

For the forward problems, $s(t)$ is calculated from $h(t)$ which represents $h_{f}(t)$ or $h_{s}(t)$. There exists analytical solutions of $s(t)$ by Green's functions [4]. The Green's function $G$ is the solution of the equation $L G=\delta$, where $L$ is the linear differential operator and $\delta$ is the Dirac's delta function. For one-dimensional heat conduction equation, $L=\partial_{t}-\alpha \partial_{x}^{2}$. If the differential equation is $L u=f$, then

$$
\begin{equation*}
L\left[\int G(x, \xi) f(\xi) d \xi\right]=\int L G(x, \xi) f(\xi) d \xi=\int \delta(x-\xi) f(\xi) d \xi=f(x) \tag{2.6}
\end{equation*}
$$

Therefore, $u=\int G(x, \xi) f(\xi) d \xi$ is a solution and it is unique in the problem concerned [4]. The solutions of the forward problems can be obtained by Green's functions. See A. 3 for more details. For equation (2.1) with the initial condition (2.2) and the first kind boundary condition (2.3),

$$
\begin{equation*}
s_{f}(t)=u(1, t)=\frac{1}{2 \sqrt{\pi}} \int_{0}^{t} \frac{e^{-1 / 4(t-\tau)}}{(t-\tau)^{3 / 2}} h_{f}(t) d \tau \equiv \mathscr{L}_{f} h_{f} . \tag{2.7}
\end{equation*}
$$

And with the second kind boundary condition (2.4),

$$
\begin{equation*}
s_{s}(t)=u(1, t)=-\int_{0}^{t} \frac{e^{-1 / 4(t-\tau)}}{\sqrt{\pi(t-\tau)}} h_{s}(\tau) d \tau \equiv \mathscr{L}_{s} h_{s} \tag{2.8}
\end{equation*}
$$

Where $\mathscr{L}_{f}$ and $\mathscr{L}_{s}$ are integral operators. The finite difference methods are also used to validate the solutions of the forward problems. See A. 4 for more details. And the results are shown in section 2.3.

### 2.2 Numerical methods for inverse problems

For the inverse problems, $s(t)$ is given to recover $h(t)$. The method mentioned in this section is from [7]. This method is called collocation method. First, the models of the forward problems are constructed. Consider $h(t)$ in a finite interval $[0, T]$. The interval is discretized into $\eta$ segmentations. Set nodes $\left\{t_{i}=i \Delta t\right\}$ where $i=0,1,2, \ldots, \eta$ and the size of time step $\Delta t=\frac{T}{\eta}$. Define

$$
\phi_{j}(t)= \begin{cases}1, & \text { if } t_{j-1} \leq t<t_{j}  \tag{2.9}\\ 0, & \text { otherwise }\end{cases}
$$

The approximation $h^{*}(t)$ of $h(t)$ is chosen to be piecewise constant.

$$
\begin{equation*}
h^{*}(t)=\sum_{j=1}^{n} h_{j} \phi_{j}(t), \tag{2.10}
\end{equation*}
$$

where $h_{j}$ are real numbers. From equation (2.7) or (2.8),

$$
\begin{equation*}
s^{*}\left(t_{i}\right)=\mathscr{L} h^{*}\left(t_{i}\right)=\sum_{j=1}^{\eta} h_{j} \mathscr{L} \phi_{j}\left(t_{i}\right)=\sum_{j=1}^{\eta} h_{j} \psi_{j}\left(t_{i}\right), \tag{2.11}
\end{equation*}
$$

where $s^{*}$ is the discretized form of $s_{f}$ or $s_{s}, \mathscr{L}$ represents the integral operator $\mathscr{L}_{f}$ in equation (2.7) or $\mathscr{L}_{s}$ in equation (2.8), $i=1,2, \ldots, \eta$ and $\psi_{j}\left(t_{i}\right)$ can be calculated from $\mathscr{L} \phi_{j}\left(t_{i}\right)$. For the first kind boundary condition (2.3),

$$
\begin{equation*}
\psi_{j}\left(t_{i}\right)=\mathscr{L}_{f} \phi_{j}\left(t_{i}\right)=\left.\operatorname{erf}\left(\frac{1}{2 \sqrt{t}}\right)\right|_{t_{i}-t_{j-1}} ^{t_{i}-t_{j}}, \tag{2.12}
\end{equation*}
$$

where erf $(x)=\frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-u^{2}} d u$. For the second kind boundary condition (2.4), from [7]

$$
\begin{equation*}
\psi_{j}\left(t_{i}\right)=\mathscr{L}_{s} \phi_{j}\left(t_{i}\right)=-\left.\left[\frac{2}{\sqrt{t}} e^{-1 / 4 t}-\left(1-\operatorname{erf}\left(\frac{1}{2 \sqrt{t}}\right)\right)\right]\right|_{t_{i}-t_{j-1}} ^{t_{i}-t_{j}} \tag{2.13}
\end{equation*}
$$

The problem can be transformed to the finite dimension linear system:

$$
\begin{equation*}
C_{\eta} h_{\eta}^{c}=s_{\eta}^{c}, \tag{2.14}
\end{equation*}
$$

where

$$
C_{\eta}=\left[\begin{array}{cccc}
\psi_{1}\left(t_{1}\right) & 0 & \cdots & 0 \\
\psi_{1}\left(t_{2}\right) & \psi_{2}\left(t_{2}\right) & \cdots & 0 \\
\vdots & & \ddots & \vdots \\
\psi_{1}\left(t_{\eta}\right) & \psi_{2}\left(t_{\eta}\right) & \cdots & \psi_{\eta}\left(t_{\eta}\right)
\end{array}\right], \quad h_{\eta}^{c}=\left[\begin{array}{c}
h_{1}^{c} \\
h_{2}^{c} \\
\vdots \\
h_{\eta}^{c}
\end{array}\right] \text { and } s_{\eta}^{c}=\left[\begin{array}{c}
s_{1}^{c} \\
s_{2}^{c} \\
\vdots \\
s_{\eta}^{c}
\end{array}\right] .
$$

For inverse problem, the elements of $C_{\eta}$ are calculated by equation (2.12) or equation (2.13) and $s_{\eta}^{c}$ is given. The goal is to recover $h_{\eta}^{c}$. Since $C_{\eta}$ is a lower triangular matrix, it can be solved directly, but the results are worse. TSVD helps to find the more stable solution.

### 2.3 Numerical results

In this section, some numerical results are demonstrated.

Example 2.1. Consider the heat equation (2.1) with the initial condition (2.2) and the first kind boundary condition (2.3) where

$$
\begin{equation*}
h_{f}(t)=-t^{2}+3 t . \tag{2.15}
\end{equation*}
$$

The temperature is measured in $t \in[0,2]$. For finite difference methods, $M=10$ and $x_{M}=5$ are selected. Another parameter $N$ is chosen to lead $\gamma$ to approach $1 / 4$. The results of the forward problem by two methods are shown in Fig. 2.1. The horizontal axis is time $t$ and the vertical axis is $s(t)$. The results from two methods are close to each other. So the solution of $s(t)$ is credible.

For inverse problem, the elements of $C_{\eta}$ are calculated by equation (2.12) and $s_{\eta}^{c}$ is from the solutions of the forward problem by Green's functions. The results are shown in Fig. 2.2 where $\eta=50$. The horizontal axis is time $t$ and the vertical axis is $h(t)$. The blue curves are the real causes and the red curves are from inverse calculations. The left is the result without any regularization and it is solved directly by $C_{\eta} \backslash s_{\eta}^{c}$ in matlab. The solution is unstable obviously. The rest parts in the figure are solved by TSVD with different cut-off levels $\mu . \sigma_{1}$ is the maximum singular value of the matrix $C_{\eta}$ and $k$ is the number of singular values which are used in calculating. $\sigma_{1} / \mu$ roughly equals to the condition number of $C_{\eta}^{*}$ in each case where $C_{\eta}^{*}$ is the approximation of $C_{\eta}$ by TSVD. From Fig. 2.2, the trend of $h_{f}(T)$ can be recovered, but the results oscillate especially when $\mu / \sigma_{1}=10^{-3}$ or $10^{-2}$.

Example 2.2. Consider the heat equation (2.1) with the initial condition (2.2) and the second kind boundary condition (2.4) where

$$
h_{s}(t)= \begin{cases}1, & \text { if } t \in[0.2,0.4] \cup[1,1.2],  \tag{2.16}\\ 0, & \text { otherwise }\end{cases}
$$

The temperature is measured in $t \in[0,2]$. For finite difference methods, $M=20$ and $x_{M}=5$ are selected. Another parameter $N$ is chosen to lead $\gamma$ to approach $1 / 4$. The results of the forward problem by two methods are shown in Fig. 2.3. And the results of the inverse problem are shown in Fig. 2.4 where $\eta=50$. All formats of the figures are the same as example 2.1. The solution of $s(t)$ can be trusted since the results from two methods are close to each other. The result without any regularization is not stable neither. The trend of $h_{s}(T)$ can also be recovered, but the results oscillate as well.


Figure 2.1: The numerical results of the forward problem for example 2.1.


Figure 2.2: The numerical results of the inverse problem for example 2.1.


Figure 2.3: The numerical results of the forward problem for example 2.2.


Figure 2.4: The numerical results of the inverse problem for example 2.2.

## Chapter 3

## Heat conduction problems in finite domain

In this chapter, the heat conduction equation in finite domain is considered.

$$
\begin{equation*}
u_{t}-\alpha u_{x x}=0, \quad 0<x<L, \quad t>0 . \tag{3.1}
\end{equation*}
$$

The initial condition is the cause in this chapter and it is

$$
\begin{equation*}
u(x, 0)=f(x) . \tag{3.2}
\end{equation*}
$$

Four different boundary conditions are used:

1. Dirichlet boundary condition is

$$
\begin{equation*}
u(0, t)=0, \quad u(L, t)=0, \quad t>0 . \tag{3.3}
\end{equation*}
$$

2. Neumann boundary condition is

$$
\begin{equation*}
u_{x}(0, t)=0, \quad u_{x}(L, t)=0, \quad t>0 \tag{3.4}
\end{equation*}
$$

3. Mixed boundary condition case 1 is

$$
\begin{equation*}
u(0, t)=0, \quad u_{x}(L, t)=0, \quad t>0 . \tag{3.5}
\end{equation*}
$$

4. Mixed boundary condition case 2 is

$$
\begin{equation*}
u_{x}(0, t)=0, \quad u(L, t)=0, \quad t>0 . \tag{3.6}
\end{equation*}
$$

For $t=T$, the temperature distribution is $g(x)$ which is the effect.

$$
\begin{equation*}
u(x, T)=g(x) \tag{3.7}
\end{equation*}
$$

The schematic diagram of the problem in this chapter is shown in Fig. 1.2 (a).

### 3.1 Methods for forward problems

For the forward problems, $g(x)$ is calculated from $f(x)$. Separation of variables can be used to find the analytic solution in this domain. See A. 5 for more details. From A.5,

$$
\begin{equation*}
g(x)=u(x, T)=\int_{0}^{L} K(x, y, T) f(y) d y . \tag{3.8}
\end{equation*}
$$

where $K(x, y, T)$ depends on the boundary condition.

1. For Dirichlet boundary condition, it is

$$
\begin{equation*}
K_{1}(x, y, T)=\frac{2}{L} \sum_{v=1}^{\infty} e^{-\left(\frac{v \pi}{L}\right)^{2} \alpha T} \sin \left(\frac{\nu \pi x}{L}\right) \sin \left(\frac{\nu \pi y}{L}\right) . \tag{3.9}
\end{equation*}
$$

2. For Neumann boundary condition, it is

$$
\begin{equation*}
K_{2}(x, y, T)=\frac{1}{L}+\frac{2}{L} \sum_{v=1}^{\infty} e^{-\left(\frac{v \pi}{L}\right)^{2} \alpha T} \cos \left(\frac{v \pi x}{L}\right) \cos \left(\frac{v \pi y}{L}\right) . \tag{3.10}
\end{equation*}
$$

3. For mixed boundary condition case 1 , it is

$$
\begin{equation*}
K_{3}(x, y, T)=\frac{2}{L} \sum_{v=1}^{\infty} e^{-\left(\frac{(v-1 / 2) \pi}{L}\right)^{2} \alpha T} \sin \left(\frac{(v-1 / 2) \pi x}{L}\right) \sin \left(\frac{(v-1 / 2) \pi y}{L}\right) . \tag{3.11}
\end{equation*}
$$

4. For mixed boundary condition case 2 , it is

$$
\begin{equation*}
K_{4}(x, y, T)=\frac{2}{L} \sum_{v=1}^{\infty} e^{-\left(\frac{(v-1 / 2) \pi}{L}\right)^{2} \alpha T} \cos \left(\frac{(v-1 / 2) \pi x}{L}\right) \cos \left(\frac{(v-1 / 2) \pi y}{L}\right) . \tag{3.12}
\end{equation*}
$$

### 3.2 Numerical methods for inverse problems

For the inverse problems, $g(x)$ is given to recover $f(x)$. The method in this section is from [8]. The trapezoid rule is used to find the numerical integration (3.8) of $g(x)$. The size of space segmentations is $\Delta y=\frac{L}{N}$. Let $x_{0}=y_{0}=0, x_{N}=y_{N}=L$, and $x_{i}=i \Delta y$ $y_{j}=j \Delta y$. Denote $g\left(x_{i}\right)$ as $g_{i}, f\left(y_{j}\right)$ as $f_{j}$ and $K\left(x_{i}, y_{j}, T\right)$ as $K_{i j}$. With the trapezoid rule,

$$
\begin{equation*}
g_{i} \approx \Delta y\left[\frac{1}{2} K_{i 0} f_{0}+K_{i 1} f_{1}+\ldots+K_{i(N-1)} f_{N-1}+\frac{1}{2} K_{i N} f_{N}\right] \tag{3.13}
\end{equation*}
$$

where $i=0,1,2, \cdots, N$ and $N$ is the number of segmentations. Thus, the problem can be transformed to the finite dimension linear system:

$$
\begin{equation*}
\widehat{K} F=G \tag{3.14}
\end{equation*}
$$

where

$$
\widehat{K}=\Delta y\left[\begin{array}{cccc}
\frac{1}{2} K_{00} & K_{01} & \cdots & \frac{1}{2} K_{0 N} \\
\frac{1}{2} K_{10} & K_{11} & \cdots & \frac{1}{2} K_{1 N} \\
\vdots & & \ddots & \vdots \\
\frac{1}{2} K_{N 0} & K_{N 1} & \cdots & \frac{1}{2} K_{N N}
\end{array}\right], \quad F=\left[\begin{array}{c}
f_{0} \\
f_{1} \\
\vdots \\
f_{N}
\end{array}\right] \text { and } \quad G=\left[\begin{array}{c}
g_{0} \\
g_{1} \\
\vdots \\
g_{N}
\end{array}\right] .
$$

Since $K(x, y, T)$ has infinite many terms, it can not be calculated numerically. But it is convergent. For convenience, the sum of $K(x, y, T)$ is limited to a finite number of expansion terms 100. For Dirichlet boundary condition,

$$
\begin{equation*}
K_{1}(x, y, T) \approx \frac{2}{L} \sum_{v=1}^{100} e^{-\left(\frac{v \pi}{L}\right)^{2} \alpha T} \sin \left(\frac{v \pi x}{L}\right) \sin \left(\frac{v \pi y}{L}\right) . \tag{3.15}
\end{equation*}
$$

For inverse problems, $G$ is known from the given temperature distribution $g(x) . \widehat{K}$ can be calculated from the expansion shown above. The problem is to find the solution of $F$. Since $\widehat{K}$ is ill-conditioned, TSVD is also applied to solve the problem. The following are some examples.

### 3.3 Numerical results

In this section, some numerical results are demonstrated.
Example 3.1. Consider the heat equation (3.1) with initial condition equation (3.2) and Dirichlet boundary condition equation (3.3) where $\alpha=L=1, f(x)=\sin (\pi x)$ and $T=1$ in equation (3.7). The analytical solution is

$$
\begin{equation*}
g(x)=\sin (\pi x) e^{-\pi^{2}} \tag{3.16}
\end{equation*}
$$

The result is shown in Fig. 3.1 where $n=20$.
Example 3.2. Consider the heat equation (3.1) with initial condition equation (3.2) and Dirichlet boundary condition equation (3.3) where $\alpha=0.01, L=1, f(x)=2 x, x \in[0,0.5]$ or $-2(x-1), x \in(0.5,1]$ and $T=1$ in equation (3.7). The analytical solution is

$$
\begin{equation*}
g(x)=\sum_{n=1}^{\infty} \frac{8}{\pi^{2}(2 n-1)^{2}} \cos \left(\frac{(2 n-1) \pi(2 x-1)}{2}\right) e^{-0.01 \pi^{2}(2 n-1)^{2} t} . \tag{3.17}
\end{equation*}
$$

Use 100 terms to approximate $g(x)$. The result is shown in Fig. 3.2 where $n=20$.


Figure 3.1: The numerical results for example 3.1.

$$
\mu / \sigma_{1}=0.0001 \text { and } \mathrm{k}=9 \quad \mu / \sigma_{1}=0.001 \text { and } \mathrm{k}=8
$$






Figure 3.2: The numerical results for example 3.2.

Example 3.3. Consider the heat equation (3.1), initial condition equation (3.2) and Dirichlet boundary condition equation (3.3) where $\alpha=0.01, L=1, f(x)=\sin (\pi x)+$ $0.1 \sin (4 \pi x)+0.2 \sin (9 \pi x)$ and $T=1$ in equation (3.7). The analytical solution is

$$
\begin{equation*}
g(x)=\sin (\pi x) \times e^{-0.01 \pi^{2}}+0.1 \sin (4 \pi x) \times e^{-0.16 \pi^{2}}+0.2 \sin (9 \pi x) \times e^{-0.81 \pi^{2}} \tag{3.18}
\end{equation*}
$$

The result is shown in Fig. 3.3 where $n=40$.
Example 3.4. Consider the heat equation (3.1), initial condition equation (3.2) and Dirichlet boundary condition equation (3.3) where $\alpha=0.01, L=1, f(x)=-x^{2}+x$ and $T=1$ in equation (3.7). The analytical solution is

$$
\begin{equation*}
g(x)=\frac{8}{\pi^{3}} \sum_{n=1}^{\infty} \sin [(2 n-1) \pi x] e^{-0.01(2 k-1)^{2} \pi^{2} t} \tag{3.19}
\end{equation*}
$$

Use 100 terms to approximate $g(x)$. The result is shown in Fig. 3.4 where $n=40$.
Example 3.5. Consider the heat equation (3.1), initial condition equation (3.2) and Neumann boundary condition equation (3.4) where $\alpha=L=1, f(x)=\cos (\pi x)$ and $T=1$ in equation (3.7). The analytical solution is $g(x)=\cos (\pi x) e^{-\pi^{2}}$. The result is shown in Fig. 3.5 where $n=20$.

Example 3.6. Consider the heat equation (3.1), initial condition equation (3.2) and the mixed boundary condition case 1 equation (3.5) where $\alpha=L=1, f(x)=\sin \left(\frac{1}{2} \pi x\right)$ and $T=1$ in equation (3.7). The analytical solution is $g(x)=\sin \left(\frac{1}{2} \pi x\right) e^{-\left(\frac{1}{2} \pi\right)^{2}}$. The result is shown in Fig. 3.6 where $n=20$.

Example 3.7. Consider the heat equation (3.1), initial condition equation (3.2) and the mixed boundary condition case 2 equation (3.6) where $\alpha=L=1, f(x)=\cos \left(\frac{1}{2} \pi x\right)$ and $T=1$ in equation (3.7). The analytical solution is $g(x)=\cos \left(\frac{1}{2} \pi x\right) e^{-\left(\frac{1}{2} \pi\right)^{2}}$. The result is shown in Fig. 3.7 where $n=20$.

In these figures, the horizontal axis is $x$ and the vertical axis is $f(x)$. The blue curves are the real causes and the red curves are from inverse calculations. The results are solved by TSVD with different cut-off levels $\mu . \sigma_{1}$ is the maximum singular value of the matrix $\widehat{K}$ and $k$ is the number of singular values which are used in calculating. The trend of $f(x)$ can be recovered, but the results perform worse when the real causes have kink points or are not smooth enough. Besides, The endpoints in Fig. 3.5, 3.6 and 3.7 are unexpected. These phenomenons may be due to Dirichlet's theorem for one-dimensional Fourier series.
$\mu / \sigma_{1}=0.0001$ and $k=9$

$$
\mu / \sigma_{1}=0.001 \text { and } k=8
$$






Figure 3.3: The numerical results for example 3.3.


Figure 3.4: The numerical results for example 3.4.


Figure 3.5: The numerical results for example 3.5.


Figure 3.6: The numerical results for example 3.6.


Figure 3.7: The numerical results for example 3.7.

## Chapter 4

## Conclusion

### 4.1 Thesis summary

The inverse heat conduction problems are studied in this thesis. There are analytical solutions to the forward problems concerned. They can be solved by Green's functions or separation of variables. It is motivated by these methods to construct the models of the forward problems. The models are discretized to the finite dimensions linear systems by discretizing the function $h(t)$ or using numerical integral. Since the problems are ill-posed, TSVD is used to find more stable solutions. These inverse heat conduction problems can be applied to fire identification (recovering the initial condition) or temperature detecting of motors (finding the boundary condition).

### 4.2 Future works

In future works, two-dimensional heat conduction problems can be considered. In addition, the parameter $\alpha$ is set as a function of the position $x$ and the temperature $u$. Further, the heat conduction equations are changed to others equations.

## Appendix A

## Supplementary materials

## A. 1 Condition numbers

If $x=\left[x_{1}, x_{2}, \ldots, x_{n}\right]^{T} \in \mathbf{R}^{n}$ is a vector and $\|x\|$ is some norm of $x$, such as $p$-norm of $x$ which is $\|x\|_{p}:=\left(\sum_{i=1}^{n}\left|x_{i}\right|^{p}\right)^{1 / p}$. The operator norm of matrix $A$ is defined as

$$
\begin{equation*}
\|A\|=\sup _{x \neq 0} \frac{\|A x\|}{\|x\|}=\sup _{\|x\|=1}\|A x\| . \tag{A.1}
\end{equation*}
$$

Assume $x^{*} \in \mathbf{R}^{n}$ be a numerical solution of the system $A x=b$ where $A \in \mathbf{R}^{m \times n}$ and $b \in \mathbf{R}^{m}$. From $H_{1}^{*}$ and $H_{2}^{*}$ in section 1.1, $m$ is equal to $n$. Define the residual vector $r^{*}$ as $b-A x^{*}$. Suppose relative residual $\rho\left(x^{*}\right)$ is controlled by $\varepsilon_{c}$ which is the precision in computer systems.

$$
\begin{equation*}
\rho\left(x^{*}\right)=\frac{\left\|r^{*}\right\|}{\|b\|}=\frac{\left\|b-A x^{*}\right\|}{\|b\|}=\frac{\left\|A x-A x^{*}\right\|}{\|A x\|} \leq \varepsilon_{c}, \tag{A.2}
\end{equation*}
$$

The relative error $\varepsilon\left(x^{*}\right)$ bound is obtained by

$$
\begin{equation*}
\varepsilon\left(x^{*}\right)=\frac{\left\|x^{*}-x\right\|}{\|x\|}=\frac{\left\|-A^{-1} r^{*}\right\|}{\|x\|} \leq \frac{\left\|A^{-1}\right\|\|A\|\left\|r^{*}\right\|}{\|A\|\|x\|} \leq \frac{\kappa(A)\left\|r^{*}\right\|}{\|A x\|}=\frac{\kappa(A)\left\|r^{*}\right\|}{\|b\|}, \tag{A.3}
\end{equation*}
$$

where $\kappa(A)=\left\|A^{-1}\right\|\|A\|$ is defined as the condition number of $A$. If two-norm $\|x\|_{2}=$ $(x \cdot x)^{1 / 2}$ is used, then $\kappa(A)=\frac{\sigma_{\max }(A)}{\sigma_{\min }(A)}$ is the ratio of the maximum singular value $\sigma_{\max }(A)$ and the minimum singular value $\sigma_{\min }(A)$. On the other hand,

$$
\begin{equation*}
\varepsilon\left(x^{*}\right)=\frac{\left\|x^{*}-x\right\|}{\|x\|}=\frac{\|A\|\left\|-A^{-1} r^{*}\right\|}{\|A\|\|x\|} \geq \frac{\left\|A\left(A^{-1} r^{*}\right)\right\|}{\|A\|\left\|A^{-1} b\right\|} \geq \frac{\left\|r^{*}\right\|}{\|A\|\left\|A^{-1}\right\|\|b\|} . \tag{A.4}
\end{equation*}
$$

Therefore, the result is

$$
\begin{equation*}
\frac{\rho\left(x^{*}\right)}{\kappa(A)} \leq \varepsilon\left(x^{*}\right) \leq \kappa(A) \rho\left(x^{*}\right) \leq \kappa(A) \varepsilon_{c} \tag{A.5}
\end{equation*}
$$

## A. 2 Truncated singular value decomposition

If $A=U \Sigma V^{T}$ is the singular value decomposition (SVD) of $A$, where $U, V \in \mathbf{R}^{n \times n}$ are orthogonal matrices and $\Sigma=\operatorname{diag}\left(\sigma_{i}\right) \in \mathbf{R}^{n \times n}$ is a diagonal matrix with $\sigma_{1} \geq \sigma_{2} \geq$ $\cdots \geq \sigma_{n} \geq 0$, where $\sigma_{i}$ are singular values of $A$ and $i=1,2, \cdots, n$. Let $k=\max \left\{i \mid \sigma_{i} \geq\right.$ $\mu\}$, where $\mu$ is the cut-off level. Choose $\Sigma_{k}=\operatorname{diag}\left(\sigma_{1}, \cdots, \sigma_{k}, 0, \cdots, 0\right)$, then $\Sigma_{k}^{+}=$ $\operatorname{diag}\left(\frac{1}{\sigma_{i}}, \cdots, \frac{1}{\sigma_{k}}, 0, \cdots, 0\right)$ is the pseudo inverse of $\Sigma_{k}$. Take

$$
\begin{equation*}
A_{k}=U \Sigma_{k} V^{T}=\underset{\operatorname{rank}(B)=k}{\operatorname{argmin}}\|A-B\|_{2} . \tag{A.6}
\end{equation*}
$$

By Eckart-Young-Mirsky theorem [1][5], the matrix $A_{k}$ is the closest approximation to $A$ that can be achieved by a matrix of rank $k$. Since $k \leq n, A_{k}$ may not be invertible. The inverse is replaced with the Moore-Penrose inverse $A_{k}^{+}$. Thus, the solution of equation (1.3) by TSVD method is

$$
\begin{equation*}
x \approx A_{k}^{+} b=\left(V \Sigma_{k}^{+} U^{T}\right) b . \tag{A.7}
\end{equation*}
$$

## A. 3 Green's functions

The texts in this section are from [4]. Consider the heat conduction equation with $\alpha=1$ and firis kind BC.

$$
\begin{aligned}
u_{t}-u_{x x} & =\delta(x-\xi) \delta(t), \quad \xi>0 \\
u\left(x, 0^{-}\right) & =0 \\
u(0, t) & =0, \quad t>0 \\
u(x, t) & \rightarrow 0 \quad \text { as } \quad x \rightarrow \infty
\end{aligned}
$$

The Green's function is

$$
\begin{equation*}
G_{1}(x, \xi, t)=\frac{1}{2 \sqrt{\pi t}}\left[e^{-(x-\xi)^{2} / 4 t}-e^{(x+\xi)^{2} / 4 t}\right] \tag{A.8}
\end{equation*}
$$

Consider the inhomogeneous equation,

$$
\begin{aligned}
u_{t}-u_{x x} & =p(x, t), \quad x \geq 0, \quad t \geq 0 \\
u\left(x, 0^{-}\right) & =0 \\
u(0, t) & =0
\end{aligned}
$$

The solution is

$$
\begin{equation*}
u(x, t)=\int_{0^{-}}^{t} d \tau \int_{0}^{\infty} p(\xi, \tau) G_{1}(x, \xi, t-\tau) d \xi \tag{A.9}
\end{equation*}
$$

Consider the homogeneous equation with nonzero initial condition,

$$
\begin{aligned}
u_{t}-u_{x x} & =0, \quad x \geq 0, \quad t \geq 0, \\
u\left(x, 0^{+}\right) & =f(x) \\
u(0, t) & =0
\end{aligned}
$$

This is equivalent to

$$
\begin{aligned}
u_{t}-u_{x x} & =\delta(t) f(x), \quad x \geq 0, \quad t \geq 0 \\
u\left(x, 0^{-}\right) & =0 \\
u(0, t) & =0
\end{aligned}
$$

The solution of $u(x, t)$ can be calculated from equation (A.9) .
Consider the inhomogeneous equation with nonzero initial condition,

$$
\begin{aligned}
u_{t}-u_{x x} & =p(x, t), \quad x \geq 0, \quad t \geq 0 \\
u\left(x, 0^{+}\right) & =f(x) \\
u(0, t) & =0
\end{aligned}
$$

The solution of $u(x, t)$ is sum of the solutions of two problems below:

$$
\begin{aligned}
& u_{t}-u_{x x}=p(x, t), x \geq 0, t \geq 0, \\
& u\left(x, 0^{-}\right)=0 \\
& u(0, t)=0 \\
& u_{t}-u_{x x}=0, x \geq 0, t \geq 0, \\
& u\left(x, 0^{+}\right)=f(x) \\
& u(0, t)=0 .
\end{aligned}
$$

Consider the homogeneous equation with nonzero boundary condition,

$$
\begin{aligned}
u_{t}-u_{x x} & =0, \quad x \geq 0, \quad t \geq 0, \\
u\left(x, 0^{+}\right) & =0 \\
u(0, t) & =h_{f}(t)
\end{aligned}
$$

Let $w(x, t)=u(x, t)-h_{f}(t)$, then

$$
\begin{aligned}
w_{t}-w_{x x} & =-\dot{h_{f}}(t)-h_{f}\left(0^{+}\right) \boldsymbol{\delta}(t) \\
w\left(x, 0^{+}\right) & =0 \\
w(0, t) & =0
\end{aligned}
$$

where $\dot{h_{f}}(t)=\frac{d h_{f}}{d t}$. The solution of $w(x, t)$ can be calculated from equation (A.9).

Consider the heat conduction equation with $\alpha=1$ and second kind BC.

$$
\begin{aligned}
& u_{t}-u_{x x}=\delta(x-\xi) \delta(t), \quad \xi>0, \\
& u\left(x, 0^{-}\right)=0 \\
& u_{x}(0, t)=0, \quad t>0, \\
& u_{x}(x, t) \rightarrow 0 \quad \text { as } \quad x \rightarrow \infty .
\end{aligned}
$$

The Green's function is

$$
\begin{equation*}
G_{2}(x, \xi, t)=\frac{1}{2 \sqrt{\pi t}}\left[e^{-(x-\xi)^{2} / 4 t}+e^{(x+\xi)^{2} / 4 t}\right] . \tag{A.10}
\end{equation*}
$$

Consider inhomogeneous equation

$$
\begin{aligned}
& u_{t}-u_{x x}=p(x, t), \quad x \geq 0, \quad t \geq 0 \\
& u\left(x, 0^{-}\right)=0 \\
& u_{x}(0, t)=0
\end{aligned}
$$

The solution is

$$
\begin{equation*}
u(x, t)=\int_{0^{-}}^{t} d \tau \int_{0}^{\infty} p(\xi, \tau) G_{2}(x, \xi, t-\tau) d \xi \tag{A.11}
\end{equation*}
$$

Consider the homogeneous equation with nonzero boundary condition

$$
\begin{aligned}
u_{t}-u_{x x} & =0, \quad x \geq 0, \quad t \geq 0 \\
u\left(x, 0^{+}\right) & =0 \\
u_{x}(0, t) & =h_{s}(t)
\end{aligned}
$$

Let $w(x, t)=u(x, t)-x h_{s}(t)$, then

$$
\begin{aligned}
w_{t}-w_{x x} & =-x \dot{h_{s}}(t)-x h_{s}\left(0^{+}\right) \boldsymbol{\delta}(t), \\
w\left(x, 0^{+}\right) & =0 \\
w_{x}(0, t) & =0 .
\end{aligned}
$$

where $\dot{h_{s}}(t)=\frac{d h_{s}}{d t}$. The solution of $w(x, t)$ can be calculated from equation (A.11). Thus, the analytical solution $u(x, t)$ of the heat conduction equations with nonzero boundary conditions can be obtained.

## A. 4 Finite difference methods

Let $u\left(x_{i}, t_{n}\right) \approx U_{i}^{n}$, where $x_{i}=i \Delta x, t_{n}=n \Delta t, i=0,1,2, \ldots, M, n=0,1,2, \ldots, N, \Delta x=$ $\frac{x_{M}-x_{0}}{M}$ and $\Delta t=\frac{t_{N}-t_{0}}{N} . M$ and $N$ are the numbers of segments of space and time respectively. For all $x_{i} \in$ interior points $(i=1,2, \ldots, M-1)$,

$$
\begin{equation*}
\frac{U_{i}^{n+1}-U_{i}^{n}}{\Delta t}=\frac{1}{(\Delta x)^{2}}\left(U_{i-1}^{n}-2 U_{i}^{n}+U_{i+1}^{n}\right) . \tag{A.12}
\end{equation*}
$$

The relation can be rewritten as

$$
\begin{equation*}
U_{i}^{n+1}=\gamma U_{i-1}^{n}+(1-2 \gamma) U_{i}^{n}+\gamma U_{i+1}^{n}, \tag{A.13}
\end{equation*}
$$

where $\gamma=\frac{\Delta t}{(\Delta x)^{2}}$ and this explicit method is stable whenever $\gamma \leq 1 / 2$. It should be careful to treat the boundary points. For the first kind boundary condition, $U_{0}^{n}=h_{f}\left(t_{n}\right)$ at $x_{0}=0$ is substituted in equation (A.13). And if $x_{M}$ is large enough, then the numerical boundary (far field) condition $U_{M}=0$ is considered and substituted in equation (A.13). Thus, the linear equation is

$$
\begin{equation*}
U^{n+1}=A_{f} U^{n}+z_{f}, \tag{A.14}
\end{equation*}
$$

where

$$
\begin{aligned}
U^{n+1} & =\left[\begin{array}{c}
U_{1}^{n+1} \\
U_{2}^{n+1} \\
\vdots \\
U_{M-2}^{n+1} \\
U_{M-1}^{n+1}
\end{array}\right], A_{f}=\left[\begin{array}{ccccc}
1-2 \gamma & \gamma & & & \\
\gamma & 1-2 \gamma & \gamma & & \\
& & \ddots & & \\
& & \gamma & 1-2 \gamma & \gamma \\
& & & \gamma & 1-2 \gamma
\end{array}\right], \\
U^{n} & =\left[\begin{array}{c}
U_{1}^{n} \\
U_{2}^{n} \\
\vdots \\
U_{M-2}^{n} \\
U_{M-1}^{n}
\end{array}\right], z_{f}=\left[\begin{array}{c}
\gamma h_{f}\left(t_{n}\right) \\
0 \\
\vdots \\
0
\end{array}\right] .
\end{aligned}
$$

For the second kind boundary condition, $\frac{U_{1}^{n}-U_{-1}^{n}}{2 \Delta x}=h_{s}\left(t_{n}\right)$ at $x_{0}=0$. It implies that $U_{-1}^{n}=$ $U_{1}^{n}-2 \Delta x h_{s}\left(t_{n}\right)$. The relation can be rewritten as

$$
\begin{equation*}
U_{0}^{n+1}=(1-2 \gamma) U_{0}^{n}+2 \gamma U_{1}^{n}-2 \gamma \Delta x h_{s}\left(t_{n}\right) . \tag{A.15}
\end{equation*}
$$

If $x_{M}$ is large enough, then the numerical boundary (far field) condition $\frac{U_{M+1}^{n}-U_{M-1}^{n}}{2 \Delta x}=0$ is considered. It implies that $U_{M+1}^{n}=U_{M-1}^{n}$. The relation is

$$
\begin{equation*}
U_{M}^{n+1}=2 \gamma U_{M-1}^{n}+(1-2 \gamma) U_{M}^{n} \tag{A.16}
\end{equation*}
$$

Thus, the linear equation is

$$
\begin{equation*}
U^{n+1}=A_{s} U^{n}-z_{s}, \tag{A.17}
\end{equation*}
$$

where

$$
\begin{aligned}
U^{n+1} & =\left[\begin{array}{c}
U_{0}^{n+1} \\
U_{1}^{n+1} \\
\vdots \\
U_{M-1}^{n+1} \\
U_{M}^{n+1}
\end{array}\right], A_{s}=\left[\begin{array}{ccccc}
1-2 \gamma & 2 \gamma & & \\
\gamma & 1-2 \gamma & \gamma & & \\
& & \ddots & & \\
& & \gamma & 1-2 \gamma & \gamma \\
& & & 2 \gamma & 1-2 \gamma
\end{array}\right], \\
U^{n} & =\left[\begin{array}{c}
U_{0}^{n} \\
U_{1}^{n} \\
\vdots \\
U_{M-1}^{n} \\
U_{M}^{n}
\end{array}\right], z_{s}=\left[\begin{array}{c}
2 \gamma \Delta x h_{s}\left(t_{n}\right) \\
0 \\
\vdots \\
0
\end{array}\right] .
\end{aligned}
$$

## A. 5 Separation of variables

Consider Dirichlet boundary conditions and in finite domain

$$
\begin{aligned}
u_{t}-\alpha u_{x x} & =0, \quad 0<x<L, \quad t>0, \\
u(x, 0) & =f(x), \\
u(0, t) & =0, \\
u(L, t) & =0 .
\end{aligned}
$$

Suppose $u(x, t)=X(x) T(t)$, then $\frac{T^{\prime}}{\alpha T}=\frac{X^{\prime \prime}}{X}=\lambda$ and $X(0)=X(L)=0$. Where $T^{\prime}=\frac{d T}{d t}$ and $X^{\prime \prime}=\frac{d^{2} X}{d x^{2}}$. Consider $\lambda$ is positive, 0 and negative.

1. If $\lambda=\omega_{v}^{2}$, then $T(t)=A e^{\omega_{v}^{2} \alpha t}$ and $X(x)=B \sinh \left(\omega_{v} x\right)+C \cosh \left(\omega_{v} x\right)$.
2. If $\lambda=0 \quad$, then $T(t)=A \quad$ and $X(x)=B x+C$.
3. If $\lambda=-\omega_{v}^{2}$, then $T(t)=A e^{-\omega_{v}^{2} \alpha t}$ and $X(x)=B \sin \left(\omega_{v} x\right)+C \cos \left(\omega_{v} x\right)$.

The solutions in case 1 diverge and contradict the equilibrium state in the reality. In case 2, from boundary conditions, $B=C=0$. In case 3 , from boundary conditions, $C=0$ and $\omega_{v}=\frac{v \pi}{L}$. So the analytical solution is

$$
\begin{equation*}
u(x, t)=\sum_{v=1}^{\infty} D_{v} \sin \left(\frac{v \pi x}{L}\right) e^{-\left(\frac{v \pi}{L}\right)^{2} \alpha t} . \tag{A.19}
\end{equation*}
$$

From initial condition, $D_{v}=\frac{2}{L} \int_{0}^{L} f(y) \sin \left(\frac{v \pi}{L} y\right) d y$. Suppose the function is measurable. Change the order of summation and integral, then

$$
\begin{equation*}
g(x)=u(x, T)=\int_{0}^{L} K(x, y, T) f(y) d y . \tag{A.20}
\end{equation*}
$$

For Dirichlet boundary condition,

$$
\begin{equation*}
K_{1}(x, y, T)=\frac{2}{L} \sum_{v=1}^{\infty} e^{-\left(\frac{v \pi}{L}\right)^{2} \alpha T} \sin \left(\frac{v \pi x}{L}\right) \sin \left(\frac{v \pi y}{L}\right) \tag{A.21}
\end{equation*}
$$

Similarly, for Neumann boundary condition,

$$
\begin{equation*}
K_{2}(x, y, T)=\frac{1}{L}+\frac{2}{L} \sum_{v=1}^{\infty} e^{-\left(\frac{v \pi}{L}\right)^{2} \alpha T} \cos \left(\frac{v \pi x}{L}\right) \cos \left(\frac{v \pi y}{L}\right) . \tag{A.22}
\end{equation*}
$$

For mixed boundary condition case 1 ,

$$
\begin{equation*}
K_{3}(x, y, T)=\frac{2}{L} \sum_{v=1}^{\infty} e^{-\left(\frac{(v-1 / 2) \pi}{L}\right)^{2} \alpha T} \sin \left(\frac{(v-1 / 2) \pi x}{L}\right) \sin \left(\frac{(v-1 / 2) \pi y}{L}\right) . \tag{A.23}
\end{equation*}
$$

For mixed boundary condition case 2 ,

$$
\begin{equation*}
K_{4}(x, y, T)=\frac{2}{L} \sum_{v=1}^{\infty} e^{-\left(\frac{(v-1 / 2) \pi}{L}\right)^{2} \alpha T} \cos \left(\frac{(v-1 / 2) \pi x}{L}\right) \cos \left(\frac{(v-1 / 2) \pi y}{L}\right) . \tag{A.24}
\end{equation*}
$$

## Appendix B

## Sample matlab codes

## B. 1 Example 2.2

The forward problem is shown in Fig. 2.3.
\%forward problem
$h f=@(x)$ double ( $x>=0.2 \& x<=0.4)+d o u b l e(x>=1 \& x<=1.2) ; ~ \% h$ function $h f=h \_s(t)$
$\mathrm{t} 0=0 ; \mathrm{tN}=2 ; \mathrm{x} 0=0 ; \mathrm{xM}=5 ; \mathrm{D}=1 ; \quad$ \%Set the domain considered ( D is \alpha)
$\mathrm{m}=20$; $\quad$ \%Set the number of spatial steps (FD method)
Tinitial=zeros $(\mathrm{m}+1,1)$; $\%$ Set the initial condition
\%Calculate s(t) by Green's function
$\mathrm{n}=50$; $\quad$ \%Set the number of time steps
$\mathrm{s}=\mathrm{zeros}(\mathrm{n}+1,1) ; \mathrm{s}(1)=0 ; \quad \%$ Set the initial condition $\mathrm{s}(1)$
delt=( $\mathrm{tN}-\mathrm{t} 0) / \mathrm{n}$; $\quad$ \%the size of time steps
for $\mathrm{i}=1$ : n fun=@(y) -1./sqrt(pi*y).*exp(-1./(4.*y)).*hf(i*delt-y); $s(i+1)=i n t e g r a l(f u n, t 0, i * d e l t) ;$
end
\%Calculate $s(t)$ by finite difference
delx $=(x M-x 0) / m ; \quad$ \%the size of spatial steps
$\operatorname{deltt}=(0.5 *(\operatorname{delx} 2) / D) ; n n=\operatorname{ceil}((t N-t 0) /$ deltt $) * 2 ; \quad \%$ Calculate $\backslash$ Delta $t$
deltt=( $\mathrm{tN}-\mathrm{t} 0) / \mathrm{nn} ; \quad$ \%the size of time steps

```
d=D*deltt/(delx^2); %d is \gamma
%Construct the matrix B
B=zeros(m+1); B (1, 1:2)=[1-2*d, 2*d];
for i=2:m
    B(i, (i-1):(i+1))=[d,1-2*d,d];
end
B(m+1,(m-1):(m+1))=[d, -2*d, 1+d];
%Calculate the distribution of temperature T
T=zeros(m+1,nn+1);T(:, 1)=Tinitial;
for j=2:nn+1
    T(:,j)=B * T(:,j-1);
    T(1,j)=T(1,j)-2 * d * delx * hf(deltt*(j-2));
end
\%---plot------------------------------
t=t0+[0:n]*delt;
tt=t0+[0:nn]*deltt;x_1=round(1/delx)+1;
p1=plot(t,s,'b');hold on;
p2=plot(tt,T(x_1,:),'ro');
p3=plot([t0,tN],[0,0],'k');
set(gca,'FontWeight', 'bold', 'fontsize', 18);
xlabel('t');ylabel('s(t)');
legend([p1 p2],{'using Green''s function ','using Finite Difference'},'fontsize',20
hold off;
%---plot------------------------------
```


## The inverse problem is shown in Fig. 2.4.

## \%inverse problem

$h f=@(x)$ double $(x>=0.2$ \& $x<=0.4)+$ double $(x>=1 \& x<=1.2) ; \% h$ function $h f=h \_s(t)$
$\mathrm{tO}=0 ; \mathrm{tN}=2 ; \mathrm{xO}=0 ; \mathrm{xM}=1 ; \quad \%$ Set the domain considered
$\mathrm{n}=50$; $\quad$ \%Set the number of time steps n
delt $=(\mathrm{tN}-\mathrm{t} 0) / \mathrm{n} ; \quad$ \%the size of time steps

```
%Construct the matrix C and s
C=zeros(n); }\begin{array}{ll}{\textrm{s}=\boldsymbol{zeros}(\textrm{n},1);}&{\mathrm{ %the matrix of collocation method}}\\{\mathrm{ for i=1:n}}&{\mathrm{ %discretization of s(t)}}
    for j=1:i
        C(i,j)=psif((i-j+1)*delt)-psif((i-j)*delt); %psif is psi function
    end
    fun=@(y) -1./sqrt(pi*y).*exp(-1./(4.*y)).*hf(i*delt-y); %Green's function
    s(i)=integral(fun,t0,i*delt);
end
f=C\s;
%---plot----------------------------%
subplot(2,3,[14])
fplot(hf,[0,2],'b-');hold on;
t_plot=(t0+0.5*delt:delt:tN-0.5*delt);
plot([t0,tN],[0,0],'k-',t_plot,f,'r--');xlabel('t');ylabel('h(t)');
axis([0,2,-10,10]);title(['\eta = ',num2str(n)]);
%---plot-----------------------------
%collocation method with TSVD
for j=1:4
    cutoff=10^(j-5); % cut-off level
    [U,D,V]=svd(C);de=D (1,1)*cutoff;
    k=1;
    while D(k,k) >= de
        V(:,k)=V(:,k)/D(k,k);
        k=k+1;
        if k>n
                break;
        end
    end
    k=k-1;
```

Us=U'*s;
f_svd=V(:,1:k)*Us(1:k); \%motivated by reduced forms of SVD
\%---plot----------------------------
subplot ( $2,3, j+1+f l o o r(j / 3)$ )
fplot(hf, $[0,2]$, 'b-');hold on;
plot([t0, tN], [0, 0],'k-', t_plot, f_svd,'r--');
axis([t0,tN,-0.2,1.2]);xlabel('t');ylabel('h(t)');
title(['\mu / \sigma_1 = ', num2str(cutoff),' and k = ', num2str(k)]);
\%---plot----------------------------
end

```
function y=psif(t) %psif is \psi function
y=zeros(1,length(t));
for i=1:length(t)
    if t(i)>0
        y(i)=-(2/sqrt(pi)*sqrt(t(i)).*exp(-1./(4*t(i)))-(1-erf(1./(2*sqrt(t(i))))))
    else
    y(i)=0;
    end
end
```


## B. 2 Example 3.2

The result is shown in Fig. 3.2.

```
f=@(x) 2*x.*double(x>=0 & x<=0.5)+2*(1-x).*double(x>0.5 & x<=1);
L=1;T=1;D=0.01;x0=0;xN=L;M=25;
dely=L/M;
k=@(n,x,y,t) 2/L* exp(-(n*pi).^2*D.*t/(L^2)).*sin(n*pi*x/L).*sin(n*pi*y/L);
kk=zeros(1,M+1);K=zeros(M+1,M+1);G=zeros(M+1,1);
for i=1:M+1
    for j=1:M+1
        for nn=1:100
```

```
        kk(nn)=k(nn,(i-1)*dely,(j-1)*dely,1);
    end
    K(i,j)=sum(kk);
    end
    G(i)=g2((i-1)*dely,T);
end
K(:,1)=K(:,1)/2;K(:,M)=K(:,M)/2;K=K*dely;
x_plot=(0:M)*dely;
for j=1:4
    cutoff=10^(j-5);
    [U,D,V]=svd(K); de=D (1, 1)*cutoff ;
    l=1;
    while D(l,l) >= de
        V(:, l)=V(:, l)/D(l, l);
        l=l+1;
        if l>M+1
        break;
        end
    end
    l=l-1;
    uG=U'*G;
    f_svd=V(:,1:1)*uG(1:1);
    %---plot-----------------------------%
    subplot(2, 2,j)
    fplot(f,[x0,xN],'b--');hold on;
    plot(x_plot,f_svd,'ro',[x0,xN],[0,0],'k');axis([x0, xN, 0, 1.2]);
    set(gca,'FontWeight','bold','fontsize',16);
    xlabel('x');ylabel('f(x)');
    title(['\mu / \sigma_1 = ',num2str(cutoff),' and k = ',num2str(l)]);
    %---plot----------------------------%
```

end

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