The 2D Heat Equation

— Analysis and Numerical Approaches

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1 Formulation of Problem

1.1 Physical Interpretation

We want to study how heat is conducted in a metal rod of length L over time. One end of the metal rod is at and the other end is at. The length of the metal rod is much greater than its cross-sectional radius, so we can think of heat conduction as a function of x and t.

Assuming the specific heat capacity of the metal rod is known, if we can find a function of temperature, we can know how the heat diffuses.

The rod is assumed to be adiabatic along its length, so it can only absorb or dissipate heat through the ends. This means that the temperature distribution depends only on the following three factors:

- 1. Initial temperature distribution, T(x,0)this is called initial condition.
- 2. The temperature at both ends of the metal rod T(0, t), T(L, t) is called boundary conditions.
- 3. The law of heat transfer from one point to another in the metal rod. The heat equation is a mathematical representation of this physical law.

We assume that the initial boundary value of the solved heat equation T(0,t) = T(L,t) = 0The problem of solving partial differential equations for a specific set of initial and boundary conditions is called an initial boundary value problem.

The heat equation can be derived from the conservation of energy: the time rate of change of the heat stored at a point on the metal rod is equal to the net heat flux into that point. This process fits the continuity equation. If Q is the heat at various points and V is the vector field of heat flow, then:

$$\frac{\partial Q}{\partial t} + \nabla V = 0$$

According to the second law of thermodynamics, if two identical bodies are in thermal contact, one being hotter than the other, then heat must flow from the hotter body to the cooler body at a rate proportional to the temperature difference. Therefore, V is proportional to the negative gradient of temperature, so: V = -kT where k is the thermal conductivity of the metal. In one dimension, $Q = \rho c T$, k, ρ , and c are the thermal conductivity, density, and specific heat capacity of the metal, respectively. And substituting into the expressions for V and Q yields the heat equation: $\frac{\partial T}{\partial t} - \frac{k}{\rho c} \frac{\partial^2 T}{\partial x^2} = 0$

Let $\Omega \subset \mathbb{R}^d$ be an open set with boundry $\Gamma := \partial \Omega$, set $\Omega_T = \Omega \times]0, T[, \Gamma_T := \Gamma \times]0, T[, \Gamma_T$ is called the *lateral* boundary of the cylinder Ω_T .

Consider the heat equation with τ -periodic boundary condition:

$$\begin{cases} k\partial_t u - \Delta_x u = f & \text{in } \Omega_T \\ u(x_i, t) = u(x_i + \tau, t) & \text{on } \Gamma_T \\ u(x, 0) = u_0(x) & \text{on } \Omega \times \{t = 0\} \end{cases}$$
 (1.1)

N.B. in high dimensional case, $\Delta_x u = \sum_{i=1}^{d} \frac{\partial^2 u}{\partial x_i^2} = \text{div}(\text{grad } u)$

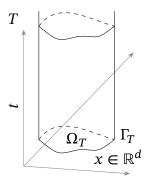


Figure 1: Region Ω_T

1.2 Fundamental Solution for Heat Equation

We observe that the heat equation involves one derivative with respect to the time variable t, and two derivatives with respect to the space variable $x_i(i=1,....n)$. At the same time ,we can observe that if u is a solution of the heat equation , $u(\lambda x, \lambda^2 t)$ for $\lambda \in \mathbb{R}$ is also a solution. So the $\frac{r^2}{t}$, (r=|x|) is very important for the heat equation. We need to find a solution as $u(x,t)=v(\frac{|x|^2}{t})(t>0,x\in\mathbb{R})$

But here we want an idea for which we can more easily find a solution (like book PDE v. Evans p 45) $u(x,t) = \frac{1}{t^a}v(\frac{x}{t^b})$ and we have x in \mathbb{R} , t > 0.

For this equation, the result 1 is easily obtained by a simple calculation.

$$\lambda^{a}u(\lambda^{b},\lambda t) = \frac{\lambda^{a}}{(\lambda t)^{a}}v(\frac{\lambda^{b}x}{(\lambda t)^{b}}) = \frac{1}{t^{a}}v(\frac{x}{t^{b}}) = u(x,t)(result1)$$

Let $\lambda = \frac{1}{t}$ and $y = \lambda^b x$, we can get v(y) = u(y, 1). We substitute u(x, t) into the first expression of the heat equation and get

$$at^{-a-1}v(y) + bt^{-a-1}y.Dv(y) + t^{-a-2b}\Delta v(y) = 0$$

To simplify the equation, we assume v(y) = w(|y|), and $w : \mathbb{R} \to \mathbb{R}$. Then the above formula becomes:

$$at^{-a-1}v(y) + bt^{-a-1}y.Dv(y) + t^{-a-2b}\Delta v(y) = aw + \frac{1}{2}rw' + w'' + \frac{n-1}{r}w' = 0$$

if we let $a = \frac{n}{2}$, we will get

$$\frac{n}{2}w + \frac{1}{2}rw' + w'' + \frac{n-1}{r}w' = (r^{n-1}w' + \frac{1}{2}r^nw)' = 0$$

 $\Rightarrow r^{n-1}w' + \frac{1}{2}r^nw = C$ and we assume that $\lim_{r\to 0} w = 0$, $\lim_{r\to 0} w' = 0$, and we can derive C = 0 and $w' = -\frac{1}{2}rw$. Thus, we have $w = de^{-\frac{r^2}{4t}}$. Finally, with $u(x,t) = \frac{1}{t^{\frac{n}{2}}}v(\frac{x}{t^{\frac{1}{2}}})$, we deduce $u(x,t) = \frac{d}{t^{\frac{n}{2}}}e^{-\frac{|x|^2}{4t}}$ So we define the basic solution of the heat equation as

♣ Definition 1.1: *The function*

$$\Phi(x,t) = \begin{cases} \frac{1}{(4\pi t)^{d/2}} e^{-\frac{|x|^2}{4t}} & x \in \mathbb{R}^d, t > 0\\ 0 & x \in \mathbb{R}^d, t < 0 \end{cases}$$
(1.2)

is called the fundamental solution of the heat equation.

The choice of the normalizing constant $(4\pi)^{-\frac{n}{2}}$ is dictated by $\int_{\mathbb{R}^n} \Phi(x,t) dx = \frac{1}{(4\pi t)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{-\frac{|x|^2}{4t}} dx = \frac{1}{\int_{\mathbb{R}^n}^n} e^{-|z|^2} dz = \frac{1}{\pi^{\frac{n}{2}}} \prod_{n=1}^{\infty} \int_{-\infty}^{+\infty} e^{-z_i^2} dz_i = 1$

1.3 Spectrum Theory and Spectral Analysis

In this part, for analysis preliminaries, [Fol99, ch.05-06] offers a panorama on the theory of L^p spaces.

Given E, F two normed vector spaces, an operator $T \in \mathcal{L}(E; F)$ is said to be copmact if the image of unit ball in E under T, i.e. $T(B_E)$ is relatively compact in F. We call an operator T is of finite rank, if dim Im $T < \infty$.

1.3.1 Riesz-Fredholm theory

- **Lemma 1.2** (Riesz): Let *E* be a normed vector space (not necessary complete), $M \subsetneq E$ a proper closed linear subspace, then $\forall \varepsilon > 0$, $\exists u \in E$ s.t. ||u|| = 1 and $d(u, M) \ge 1 \varepsilon$.
- ▶ **Theorem 1.3:** Let E be a normed vector space with compact unit ball B_E , then E is finite-dimensional.
- ▶ **Theorem 1.4** (Fredholm alternative): Let $T \in \mathcal{L}(E)$ be a compact operator, then
 - Ker(I T) is finite-dimensional.
 - Im (I T) is closed. More precisely, Im $(I T) = \text{Ker}(I T')^{\perp}$
 - $\operatorname{Ker}(I T) = \{0\} \iff \operatorname{Im}(I T) = E$
 - $\dim \operatorname{Ker}(I-T) = \dim \operatorname{Ker}(I-T')$

Proof: Admitted. [cf. Bre11, p.160-162]

\maltese Definition 1.5 (resolvent set, spectrum and eigenvalue): Let $T \in \mathcal{L}(E)$, the resolvent set, denoted by $\rho(T)$, is defined by

$$\rho(T) := \{ \lambda \in \mathbb{C}; (T - \lambda I) : E \to E \text{ is bijective } \}$$

The spectrum, denoted by $\sigma(T)$, is the complement of the resolvent set, i.e., $\sigma(T) = \mathbb{C} \setminus \rho(T)$. A complex number λ is said to be an eigenvalue of T if $Ker(T - \lambda I) \neq \{0\}$. The set of eigenvalues of T is denoted by EV(T). The space $Ker(T - \lambda I)$ is called the eigenspace of T, the elemet in it is called eigenvector.

Remark 1: If *E* is a Banach space, the open mapping theorem tells us, the bijectivity of *T* equals that $T^{-1} \in \mathcal{L}^{-1}(E)$. Actually we have following consequece:

▶ Proposition 1.6:

- If T ∈ L(E) and ||I-T|| < 1 where I is the identity operator, then T is invertible, the series lim_{n→∞} ∑_{n=0}[∞] (I − T)ⁿ = T⁻¹ in L(E).
 The set of invertible operators in L(E), denoted as GL(E), is an open set in L(E), and GL(E) →
- The set of invertible operators in $\mathcal{L}(E)$, denoted as GL(E), is an open set in $\mathcal{L}(E)$, and $GL(E) \to GL(E)$; $T \mapsto T^{-1}$ is continuous. More precisely, if $S \in GL(E)$ and $||T-S|| < ||T^{-1}||^{-1}$, then $S \in GL(E)$.

► **Theorem 1.7** (Gelfand):

- We have $\|T^n\|^{1/n} \xrightarrow{n \to \infty} \inf_n \|T^n\|^{1/n}$, we call this limite, denoted by r(T), the spectral radius of T. Moreover, $r(T) \le \|T\|$, and $\forall \lambda \in \sigma(T), |\lambda| \le r(T)$. In particular, $\sigma(T)$ is a compact set in \mathbb{C} .
- For all $T \in \mathcal{L}(E)$, we have $\sigma(T) \neq \emptyset$. Moreover

$$r(T) = \max_{\lambda \in \sigma(T)} \{|\lambda|\}$$

Proof: [cf. Lax02, p195-197]

4 Definition 1.8 (adjoint, self-adjoint): Let $A : Dom(A) \subset E \to F$ be an unbounded linear operator that is densely defined. We shall introduce an unbounded operator $A' : Dom(A') \subset F' \to E'$ as follows:

$$\operatorname{Dom}(A') := \{ v \in F' : \exists c \ge 0 \text{ s.t. } |\langle v, Au \rangle| \ge c ||u||, \quad \forall u \in \operatorname{Dom}(A) \}$$
$$_{F'} \langle v, Au \rangle_F = _{E'} \langle A'v, u \rangle_E, \quad \forall u \in \operatorname{Dom}(A), \forall v \in \operatorname{Dom}(A')$$

A bounded operator T is said to be self-adjoint if T' = T.

▶ **Theorem 1.9:** Suppose that H is a separable Hilbert space, T is a compact self-adjoint operator. then there exists a Hilbert basis composed of eigenvectors of T.

Our last statement is a fundamental result. It asserts that every compact self-adjoint operator may be diagonalized in some suitable basis.

1.3.2 Eigenfunctions and spectral decomposition

Now, we have sufficient tools to proceed the spectral analysis of heat equation. (More generally, the spectral analysis could be applied to other types of PDE [cf. Bre11, ch.08-09; Lax02, ch.33-36])

♣ Definition 1.10 (Sobolev spaces, distribution):

$$W^{m,p}(\Omega):=\left\{u\in L^p(\Omega): \partial^\alpha u\in L^p(\Omega), \forall \alpha=(\alpha_1,\dots,\alpha_d)\in\mathbb{R}^d_+ \ and \ 1\leq |\alpha|\leq d\right\}$$

For index $\alpha \in \mathbb{R}^d_+$, we note $|\alpha| = \sum_{i=1}^d \alpha_i$. The norm $\|\cdot\|_{W^{m,p}(\Omega)}$ defined by

$$||u||_{W^{m,p}(\Omega)} = \left(\sum_{|\alpha|=0}^{d} ||\partial^{\alpha} u||_{L^{2}(\Omega)}^{2}\right)^{\frac{1}{2}}$$

makes the Sobolev space $W^{m,p}(\Omega)$ complete.

We simply note $H^m(\Omega) := W^{m,2}(\Omega)$, since it's a Hilbert space. At last, we define $H_0^m(\Omega) := \overline{\mathcal{D}(\Omega)}^{H^m(\Omega)}$, that means the closure of $\mathcal{D}(\Omega)$ in $H^m(\Omega)$.

Where $\mathcal{D}(\Omega) = C_c^{\infty}(\Omega)$ called the set of test functions. Its dual space $\mathcal{D}'(\Omega)$ is called distribution.

 $H_0^1(\Omega)$ need not to inherit the norm from $H^1(\Omega)$, there is an equivalent norm inducted by the inner product:

$$\langle v, u \rangle_{H_0^1(\Omega)} = \langle \nabla u, \nabla v \rangle_{L^2(\Omega)}$$

The notion of distriburion generalized the notion of function. We could find that the Dirac mass at x = a: $\delta(x - a)$ is not a function, however, it's a distribution. Important example: $L^1_{loc}(\Omega)$ is a distribution. For more details, [cf. Gos20, ch.03-05].

▶ **Theorem 1.11** (the spectrum of Laplacian operator): Suppose $T: L^2(\Omega) \to L^2(\Omega)$; $f \mapsto u$, where u is the weak solution (i.e. solution in $H_0^1(\Omega)$) of

$$\begin{cases}
-\Delta u_f = f & \text{in } \Omega \\
u_f = 0 & \text{on } \partial\Omega
\end{cases}$$
(1.3)

Then T is compact and self-adjoint. Moreover T is positive defined.

 \triangleright *Proof*: u_f is characterized by $u_f \in H_0^1(\Omega), \forall \varphi \in H_0^1(\Omega), \int_{\Omega} \nabla u_f \nabla \varphi = \int_{\Omega} f \varphi$



 $T = i \circ S$, where S is linear continuous and $i : H_0^1(\Omega) \to L^2(\Omega)$ is compact injection (it's a result of Reillich-Kondrachov's Theorem, [cf. Bre11, ch.9.3, p.285], we don't discuss the interpolation of Sobolev space here)

To prove that T self-adjoint and positive is relatively easy, it's direct consequnce of properties of $L^2(\Omega)$.

Thus, by theorem 1.9, there exists a Hilbert basis in $L^2(\Omega)$ consists of the eigenvalues of T: assume that $\Omega \subset \mathbb{R}^d$ is a bounded open set, then there exist a Hilbert basis $\{e_n\}_n$ of $L^2(\Omega)$ s.t. $e_n \in H_0^1(\Omega) \cap C^{\infty}(\Omega), \forall n \text{ and a sequence } \{\lambda_n\}_n \text{ of real numbers with } \lambda_n > 0, \forall n \text{ and } \lambda_n \to +\infty \text{ s.t.}$

$$-\Delta e_n = \lambda_n e_n \quad \text{in } \Omega$$

We say that $\{\lambda_n\}_n$ are the eigenvalues of $-\Delta$ (with Dirichlet boundray condition) and the $\{e_n\}_n$ are the associated eigenfunctions.

► **Corollary 1.12:** $\left\{\frac{1}{\sqrt{\lambda_n}}e_n\right\}_{n}$ is a Hilbert basis for $H_0^1(\Omega)$ equipped with the inner product

$$\langle v, w \rangle_{H_0^1(\Omega)} = \int_{\Omega} \nabla v \nabla w$$

▷ *Proof:*

$$\begin{split} \left\langle \nabla \frac{1}{\sqrt{\lambda_n}} e_n, \nabla \frac{1}{\sqrt{\lambda_m}} e_m \right\rangle_{L^2(\Omega)} &= \frac{1}{\sqrt{\lambda_n}} \left\langle \sqrt{\lambda_n} \nabla T e_n, \nabla \frac{1}{\sqrt{\lambda_m}} e_m \right\rangle_{L^2(\Omega)} \\ &= \frac{1}{\sqrt{\lambda_n}} \sqrt{\lambda_n \lambda_m} \int_{\Omega} e_n e_m \\ &= \sqrt{\frac{\lambda_m}{\lambda_n}} \left\langle e_n, e_m \right\rangle_{L^2(\Omega)} = \sqrt{\frac{\lambda_m}{\lambda_n}} \delta_n^m \end{split}$$

Then $\left\langle \nabla \sqrt{\lambda_n} e_n, \nabla \sqrt{\lambda_m} e_m \right\rangle = \sqrt{\frac{\lambda_m}{\lambda_n}} \delta_n^m \implies \left\{ \sqrt{\lambda_n} e_n \right\}_n$ is an orthonomal family in $H_0^1(\Omega)$. Lastly, we should prove $\left\{ \sqrt{\lambda_n} e_n \right\}_n$ is a maximal family, i.e. it spans a dense party of $H_0^1(\Omega)$. Let $v \in H_0^1(\Omega)$ s.t. $\forall n, \left\langle \sqrt{\lambda_n} \nabla e_n, \nabla v \right\rangle_{L^2(\Omega)} = 0 \implies \frac{1}{\sqrt{\lambda_n}} \left\langle \nabla T e_n, \nabla v \right\rangle_{L^2(\Omega)} = 0 \implies \langle e_n, v \rangle_{L^2(\Omega)} = 0$. Since $\{e_n\}_n$ is a Hilbert basis of $L^2(\Omega)$, then v = 0 in $L^2(\Omega)$, naturally v = 0 in $H_0^1(\Omega)$.

We have hereby proved that $\left(\overline{\operatorname{span}(\{e_n\})}^{H_0^1(\Omega)}\right)^{\perp} = \{0\}$ in $H_0^1(\Omega)$, then $\left\{\sqrt{\lambda_n}e_n\right\}_n$ is a maximal family.

Let's begin with the Dirichlet's condition.

$$\begin{cases}
-\Delta e_i = \lambda_i e_i & \text{in } \Omega \\
e_i = 0 & \text{on } \Gamma
\end{cases}$$
(1.4)

When dim $\mathbb{R}^d=1$, we have $e_n=\sqrt{2}\sin(n\pi x)$ and $\lambda_n=n^2\pi^2$, n=1,2,... We seek for the solution of equation 1.1 in the form of series

$$u(x,t) = \sum_{i=1}^{\infty} a_i(t)e_i(x)$$
 (1.5)

The core ideal is to separate time variable. i.e.

$$u(x,t) = a(t)\phi(x), \quad \forall x = (x_1, x_2, \dots, x_d) \in \mathbb{R}^d$$

We see immediately that the function $a_i(t)$ must satisfy

$$a_i'(t) + \lambda_i a_i(t) = 0 \tag{1.6}$$

So $a_i(t) = a_i(0)e^{-\lambda_i t}$. The constant $a_i(0)$ is determined by the relation

$$u_0(x) = \sum_{i=1}^{\infty} a_i(0)e_i(x)$$
(1.7)

$$-\Delta_{x}u(t) = \sum_{i=1}^{\infty} \langle u_{0}, e_{i} \rangle_{L^{2}(\Omega)} \frac{1}{\lambda_{n}} e_{n} \quad \text{in } \mathcal{D}'(\Omega)$$
(1.8)

1.4 Maximum Principle

▶ **Theorem 1.13** (Strong maximum principle): Assume that $u \in C^2(\Omega) \cap C^1(\overline{\Omega})$ solve the heat equation in Ω_T , then

$$\max_{\overline{\Omega}_T} u = \max_{\partial \Omega_T} u \tag{1.9}$$

Theorem 1.14: Assume that $u_0 \in L^2(\Omega)$, u is the solution of the equation 1.1, then we have, for all $(x,t) \in \Omega_T$

$$\min\left\{0, \inf_{\Omega} u_0\right\} \le u(x, t) \le \max\left\{0, \sup_{\Omega} u_0\right\}$$

Proof: Instead of a classical mean value formula [cf. Eva10, ch.02.3.2-02.3.3], we use Stampacchia's truncation method. Set

$$K = \max \left\{ 0, \sup_{\Omega} u_0 \right\}$$

and assume that $K < +\infty$. Fix a function G s.t.

- $|G'(s)| \le M$, $\forall s \in \mathbb{R}$
- *G* is strictly increasing on $]0, \infty[$
- G(s) = 0, $\forall s \le 0$

and let

$$H(s) = \int_0^s G(\sigma) d\sigma, \quad s \in \mathbb{R}$$

Easy check the function φ defined by

$$\varphi(t) = \int_{\Omega} H(u(x, t) - K) \, \mathrm{d}x$$

has the following properties:

- $\varphi \in C([0, \infty[; \mathbb{R}), \varphi(0) = 0, \varphi \ge 0 \text{ on } [0, \infty[$
- $\varphi \in C^1(]0,\infty[;\mathbb{R})$

 $\varphi'(t) = \int_{\Omega} G(u(x,t) - K) \partial_t u(x,t) \, dx$ $= \int_{\Omega} G(u(x,t) - K) \Delta_x u(x,t) \, dx$ $= -\int_{\Omega} G'(u - K) |\nabla u|^2 \, dx$

since $G(u(x,t)-K)\in H^1_0(\Omega)$ for every t>0, it follows that $\varphi\equiv 0$ and thus, $\forall t>0,\ u(x,t)\leq K$ a.e. on Ω .

▶ **Theorem 1.15:** Assume $u \in C(\overline{\Omega} \times [0, T])$, u is of class C^1 in t and of class C^2 in $x \in \Omega \times]0, T[$, $\partial_t u - \Delta_x u \leq 0 \in \Omega \times]0, T[$, then

$$\max_{\overline{\Omega} \times [0,T]} u = \max_{\mathfrak{P}} u$$

where $\mathfrak{P} = (\overline{\Omega} \times \{0\}) \cup (\Gamma \times]0, T[)$ is called the **parabolic boundary** of the cylinder $\Omega \times]0, T[$

2 Numerical Approaches

2.1 Discrete and Fast Fourier Transform (DFT & FFT)

[cf. Sha03; Sch01, ch.08; Mal08, ch.03.3]

$$\widehat{f}(k) = \int_0^\tau f(x)e^{-2i\pi kx} \, \mathrm{d}x \xrightarrow{\text{discretization}} U_k = \frac{1}{N} \sum_{j=0}^{N-1} f(\frac{j}{N})e^{-2i\pi k\frac{j}{N}}$$
 (2.1)

- 2.2 Finite Difference Method (FDM) for 1D Heat Equation
- 2.3 Finite Element Method (FEM) Approximation for 1D Heat Equation
- 2.4 FDM for 2D Heat Equation
- 2.5 FEM for 2D Heat Equation
- 3 Analysis of Algorithms
- 3.1 Consistency
- 3.2 Stability
- 3.3 Order of Convergence
- 3.4 Possibility of Improvement
- 4 Application on Economics and Finance
- 4.1 The Black-Scholes PDE for Option Pricing
- 4.2 Optimal Portfolio for Consumption and Investment

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