

The 2D Heat Equation

— Analysis and Numerical Approaches

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1 Formulation and Primary Exploration 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 $x=0$ and the other end is at $x=L$. 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 $T(0, t) = T(L, t) = 0$

The 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: $V = -k \nabla T$ 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. Substituting into the expressions for V and Q yields the heat equation:

$$\frac{\partial T}{\partial t} - \frac{k}{\rho c} \frac{\partial^2 T}{\partial x^2} = 0$$

Now we give a formal formulation for the heat equation:

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

Consider the heat equation with L -periodic boundary condition:

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

N.B. where $k > 0$ is a 'diffusion coefficient'. However, since the constant can be scaled out by defining a rescaled time $\tau = t/k$ to get

$$u_\tau - \Delta u = f$$

Hence we could simplify the formulation as

$$\begin{cases} \partial_t u - \Delta u = f(x, t) & \text{in } \Omega_T \\ u(x, t) = u(x + L, t) & \text{on } \Gamma_T \\ u(x, 0) = u_0(x) & \text{on } \Omega \times \{t = 0\} \end{cases} \quad (1.2)$$

In high dimensional case, $\Delta u = \Delta_x u = \sum_1^d \frac{\partial^2 u}{\partial x_i^2} = \text{div}(\text{grad } u)$. Finally, in PDE context, we often note $\frac{\partial u}{\partial t}$ as u_t and $u_{xx} := \frac{\partial^2 u}{\partial x^2} = \Delta u$ if no ambiguity occurs.

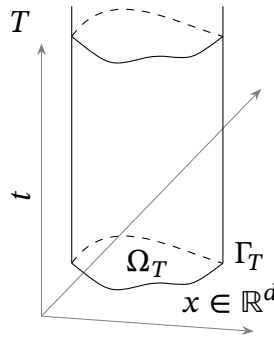


Figure 1: Region Ω_T

The Modeling Context: An Excursion to IV and BCs

1. **Dirichlet:** The temperature is fixed at the boundary
2. **Neumann:** The end is insulated (no heat enters or escapes).
3. **Robin:** Some heat enters or escapes, with an amount proportional to the temperature:

$$\alpha u = -\beta \frac{\partial u}{\partial n}$$

where $\frac{\partial u}{\partial n} := \nabla u \cdot \vec{n}$. For the area Ω whether heat enters or escapes the system depends on the boundary $\Gamma = \partial\Omega$. The heat flux $-\beta \frac{\partial u}{\partial n}$ is to the right if it is positive, so at the point a belongs to boundary, heat enters the system when $\alpha > 0$ and leaves when $\alpha < 0$.

4. **Periodic:** The temperature is periodic at the boundary.

The same interpretations apply when the equation is describing diffusion of some other quantity. Non-homogeneous boundary conditions can be imposed, for instance

$$u(a, t) = g(a, t), \quad a \in \Gamma_T$$

which might be used to model the ambient temperature increasing with time.

Remark 1 (Robin's BC): All BCs could be expressed as Robin's condition

$$\alpha u(a) + \beta \frac{\partial u}{\partial n}(a) = g, \quad a \in \partial\Omega$$

Dirichlet's condition means that $\beta = 0$ and Neumann's condition means that $\alpha = 0$.

Remark 2: At each point of Γ , the BCs could be different.

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 $x_i (i = 1, \dots, n)$. 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 [cf. [Eva10](#), 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.

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

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 $w : \mathbb{R} \rightarrow \mathbb{R}$. 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

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

$\Rightarrow r^{n-1}w' + \frac{1}{2}r^n w' = C$ and we assume that $\lim_{r \rightarrow 0} w = 0, \lim_{r \rightarrow 0} w' = 0$, 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

$$\Phi(x, t) = \begin{cases} \frac{1}{(4\pi t)^{d/2}} e^{-\frac{|x|^2}{4t}} & x \in \mathbb{R}^d, t > 0 \\ 0 & x \in \mathbb{R}^d, t < 0 \end{cases} \quad (1.3)$$

is called the fundamental solution of the heat equation.

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

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 compact 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 $\dim \text{Im } T < \infty$.

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 $d(u, M) \geq 1 - \varepsilon$.

► **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

- $\text{Ker}(I - T)$ is finite-dimensional.
- $\text{Im}(I - T)$ is closed. More precisely, $\text{Im}(I - T) = \text{Ker}(I - T')^\perp$
- $\text{Ker}(I - T) = \{0\} \iff \text{Im}(I - T) = E$
- $\dim \text{Ker}(I - T) = \dim \text{Ker}(I - T')$

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

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

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

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

Remark 3: 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 consequence :

► **Proposition 1.6:**

- If $T \in \mathcal{L}(E)$ and $\|I-T\| < 1$ where I is the identity operator, then T is invertible, the series $\lim_{n \rightarrow \infty} \sum_{n=0}^{\infty} (I-T)^n = T^{-1}$ in $\mathcal{L}(E)$.
- The set of invertible operators in $\mathcal{L}(E)$, denoted as $GL(E)$, is an open set in $\mathcal{L}(E)$, and $GL(E) \rightarrow GL(E); T \mapsto T^{-1}$ 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 $\|T^n\|^{1/n} \xrightarrow{n \rightarrow \infty} \inf_n \|T^n\|^{1/n}$, we call this limite, denoted by $r(T)$, the spectral radius of T . Moreover, $r(T) \leq \|T\|$, and $\forall \lambda \in \text{Spec}(T), |\lambda| \leq r(T)$. In particular, $\text{Spec}(T)$ is a compact set in \mathbb{C} .
- For all $T \in \mathcal{L}(E)$, we have $\text{Spec}(T) \neq \emptyset$. Moreover

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

▷ *Proof:* [cf. [Lax02](#), p195-197] □

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

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

$${}_{F'} \langle v, Au \rangle_F = {}_{E'} \langle A'v, u \rangle_E, \quad \forall u \in \text{Dom}(A), \forall v \in \text{Dom}(A')$$

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):

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

For index $\alpha \in \mathbb{R}_+^d$, we note $|\alpha| = \sum_1^d \alpha_i$. The norm $\|\cdot\|_{W^{m,p}(\Omega)}$ defined by

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

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 distribution 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: $L_{loc}^1(\Omega)$ is a distribution. For more details, [cf. Gos20, ch.03-05].

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

$$\begin{cases} -\Delta u_f = f & \text{in } \Omega \\ u_f = 0 & \text{on } \partial\Omega \end{cases} \quad (1.4)$$

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

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

$$\begin{array}{ccc} f & \xrightarrow{T} & u \\ & \searrow s & \uparrow i \\ & & u_f \end{array}$$

$T = i \circ S$, where S is linear continuous and $i : H_0^1(\Omega) \rightarrow L^2(\Omega)$ 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 consequence 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. $e_n \in H_0^1(\Omega) \cap C^\infty(\Omega), \forall n$ and a sequence $\{\lambda_n\}_n$ of real numbers with $\lambda_n > 0, \forall n$ and $\lambda_n \rightarrow +\infty$ 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 boundary condition) and the $\{e_n\}_n$ are the associated eigenfunctions.

▷ *Proof:* □

► **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:*

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

Then $\langle \nabla \sqrt{\lambda_n} e_n, \nabla \sqrt{\lambda_m} e_m \rangle = \sqrt{\frac{\lambda_m}{\lambda_n}} \delta_n^m \implies \{\sqrt{\lambda_n} e_n\}_n$ is an orthonormal family in $H_0^1(\Omega)$.

Lastly, we should prove $\{\sqrt{\lambda_n} e_n\}_n$ 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. $\forall n, \langle \sqrt{\lambda_n} \nabla e_n, \nabla v \rangle_{L^2(\Omega)} = 0 \implies \frac{1}{\sqrt{\lambda_n}} \langle \nabla T e_n, \nabla v \rangle_{L^2(\Omega)} = 0 \implies \langle e_n, v \rangle_{L^2(\Omega)} = 0$.

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 $\left(\overline{\text{span}(\{e_n\})}^{H_0^1(\Omega)} \right)^\perp = \{0\}$ in $H_0^1(\Omega)$, then $\{\sqrt{\lambda_n} e_n\}_n$ is a maximal family. □

However, our problem is more complicated than the case above, that's because the restriction of initial value (IV) and boundary conditions (BCs) may not allow the solution belong to $H_0^m(\Omega)$, which implies only a zero Dirichlet BC. Thus, the choice of a proper working space is the first and the crucial matter to think about.

Separation of Variables and Superposition Principle: A History

When Joseph Fourier contemplate the heat equation

As we did before, sometimes we note u_{xx} as Δu , because the Laplacian operator is a linear operator on u with respect to x — actually, the heat equat also belongs to linear PDE, which refers that

$$u_t = -L[u] + f(x, t) \quad (1.5)$$

A linear, homogeneous PDE obeys the superposition principle: u_1, u_2 are solutions $\implies c_1 u_1 + c_2 u_2$ is a solution for all scalars $c_1, c_2 \in \mathbb{R}$. The concepts of linearity and homogeneity also apply to boundary conditions, in which case the variables are evaluated at specific points.

For example, here lists the linear operators for some basic linear PDEs, i.e. heat equation, wave equation, Poisson's equation.

$$L_h = \partial_t - \partial_{xx}, \quad L_w = \partial_{tt} - \partial_{xx}, \quad L_P = \nabla^2$$

an example of non-linear PDE:

$$u_t + uu_x = u_{xx}$$

However, L_h is generally not a compact and self-adjoint operator, which means we should consider rather the Laplacian operator Δ and the basis is a series of functions involve only x .

To have an eigenfunction of the operator L , we must prescribe Ω and associated boundary conditions. Generally, we could sketch out the proper working space V as

$$V = \{f \in H^m(\Omega) : f \text{ satisfies BCs}\} \quad (1.6)$$

The eigenfunctions we need is to solve the eigenvalue problem

$$L[\phi] = \lambda\phi, \quad \phi \in V$$

By theorem 1.9, there is a sequence of eigenfunctions $\{\phi_n\}$ with eigenvalues $\{\lambda_n\}$ that form an orthogonal basis for the space V .

Now at each fixed time t , the function $u(x, t)$, regarded as a function of x , lies inside the space V . It follows that there are coefficients $a_n(t)$ such that

$$u(x, t) = \sum_{n=0}^{\infty} a_n(t) \phi_n(x) \quad (1.7)$$

Our objective now is to determine the functions $a_n(t)$. We write the heat source f in terms of eigenfunctions:

$$f(x, t) = \sum_{n=0}^{\infty} f_n(t) \phi_n(x) \quad (1.8)$$

Now substitute this 1.8 and the eigenfunction expansion for u (equation 1.8) into the PDE (30) to obtain

$$\underbrace{\sum_{n=0}^{\infty} a_n(t) \phi_n(x)}_{u_t} = \underbrace{- \sum_{n=0}^{\infty} a_n(t) \lambda_n \phi_n(x)}_{-L[u]} + \underbrace{\sum_{n=0}^{\infty} f_n(t) \phi_n(x)}_f \quad (1.9)$$

In detail, the second term was found using the eigenfunction property and linearity of L :

$$\begin{aligned} L[u] &= L \left[\sum_{n=0}^{\infty} a_n(t) \phi_n(x) \right] \\ &= \sum_{n=0}^{\infty} a_n(t) L[\phi_n(x)] \\ &= \sum_{n=0}^{\infty} a_n(t) \lambda_n \phi_n(x) \end{aligned}$$

Note that since $a_n(t)$ is only a function of t , it is constant as far as L is concerned so by linearity, $L[a_n(t) \phi_n(x)] = a_n(t) L[\phi_n(x)]$, where we have used the fact that L is linear to move.

Now we gather equation 1.9 together under the basis $\{\phi_n\}$:

$$0 = \sum_{n=0}^{\infty} \underbrace{[a'_n(t) + \lambda_n a_n(t) - f_n(t)]}_{\Psi_n(t)} \phi_n(x) = \sum_{n=0}^{\infty} \Psi_n(t) \phi_n(x)$$

Since the $\{\phi_n(x)\}$'s are a basis, the coefficient of each basis function must be zero at all times t (otherwise, the $\{\phi_n(x)\}$'s would be linearly dependent at some t), i.e. $\Psi_n(t) \equiv 0$. It follows that for each n ,

$$a'_n(t) + \lambda_n a_n(t) = f_n(t), \quad \forall n > 0, t \in]0, T] \quad (1.10)$$

This equation is a first-order linear ODE for $a_n(t)$ that is easy to solve.

To complete our problem, the last missing piece is the initial value, i.e. $a_n(0)$.

Recall we set $u(x, 0) = u_0(x)$. Write the IV in terms of eigenfunctions:

$$u_0(x) = \sum_{n=0}^{\infty} u_{0,n} \phi_n(x)$$

For the solution 1.7 satisfies the IV, we need the constants γ_n

$$\underbrace{\sum_{n=0}^{\infty} a_n(0) \phi_n(x)}_{u(x,0)} = \underbrace{\sum_{n=0}^{\infty} u_{0,n} \phi_n(x)}_{u_0(x)}$$

Again, since the $\{\phi_n(x)\}$'s are absis, the two sums must be equal term-by-term, so

$$a_n(0) = u_{0,n}, \quad \forall n$$

Finally, this condition and equation 1.10 lets us solve for a unique $a_n(t)$ (as we get a first order IV problem), which completes the process.

Sturm–Liouville Eigenvalue Problems

We have found the method of separation of variables to be quite successful in solving some homogeneous partial differential equations with homogeneous boundary conditions.

In all examples we have analyzed so far, the boundary value problem that determines the needed eigenvalues (separation constants) has involved the simple ordinary differential equation

$$\phi''(x) + \lambda \phi(x) = 0 \quad (1.11)$$

$$\frac{d}{dx} \left(p \frac{d\phi}{dx} \right) + q\phi + \lambda \sigma \phi = 0 \quad (1.12)$$

Explicit solutions of this equation determined the eigenvalues λ from the homogeneous boundary conditions.

► **Proposition 1.13:** *For any regular Sturm-Liouville problem, all of the following theorems are valid:*

1. All the eigenvalues λ are real.
2. There exist an infinite number of distinct eigenvalues:

$$\lambda_1 < \lambda_2 < \dots < \lambda_n < \dots \rightarrow +\infty$$

3. Corresponding to each eigenvalue λ_n , there is an eigenfunction, denoted $\phi_n(x)$ (which is unique to within an arbitrary multiplicative constant)

4. The eigenfunctions $\phi_n(x)$ form a “complete” set, meaning that any piecewise smooth function $f(x)$ can be represented by a generalized Fourier series of the eigenfunctions:

$$f(x) \sim \sum_{n=0}^{\infty} a_n \phi_n(x)$$

5. Eigenfunctions belonging to different eigenvalues are orthogonal relative to the weight function $\sigma(x)$. In other words,

$$\int_{\Omega} \phi_m(x) \phi_n(x) \sigma(x) dx = 0, \quad \lambda_m \neq \lambda_n$$

6. Any eigenvalue can be related to its eigenfunction by the **Rayleigh quotient**

$$\lambda = \frac{-\int_{\Gamma} p \phi \frac{\partial \phi}{\partial n} d\Gamma + \int_{\Omega} [p(\frac{d\phi}{dx})^2 - q\phi^2]}{\int_{\Omega} \phi^2 \sigma}$$

Asymptotic Behavior:

1.4 Maximum Principle

► **Theorem 1.14** (Strong maximum principle): Assume that $u \in C^2(\Omega) \cap C^1(\overline{\Omega})$ solve the heat equation in Ω_T , then

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

► **Theorem 1.15:** Assume that $u_0 \in L^2(\Omega)$, u is the solution of the equation 1.2, then we have, for all $(x, t) \in \Omega_T$

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

▷ *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.

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

and let

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

Easy to check the function φ defined by

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

has the following properties:

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

$$\begin{aligned} \varphi'(t) &= \int_{\Omega} G(u(x, t) - K) \partial_t u(x, t) \, dx \\ &= \int_{\Omega} G(u(x, t) - K) \Delta u(x, t) \, dx \\ &= - \int_{\Omega} G'(u - K) |\nabla u|^2 \, dx \\ &\leq 0 \end{aligned}$$

since $G(u(x, t) - K) \in H_0^1(\Omega)$ for every $t > 0$, it follows that $\varphi \equiv 0$ and thus, $\forall t > 0$, $u(x, t) \leq K$ a.e. on Ω . \square

► **Theorem 1.16:** 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)

In section 1.3.2 we have exhibited a complete procedure to solve heat equation in using eigenfunction's method, however, it's impossible to calculate a basis and corresponding coefficients presented by infinite series in computer. Generally we calculate a sufficient large number of finite items to approach the infinite series.

Let's start with a concrete example in 1D spacetime .

$$\begin{cases} \partial_t u - 2tu_{xx} = e^{-t^2} \sin x & \text{in }]0, \pi[\times]0, 1[\\ u(0, t) = u(\pi, t) & \text{on } \{0, \pi\} \times]0, 1[\\ u(x, 0) = 3 \sin 2x & \text{on }]0, \pi[\times \{t = 0\} \end{cases} \quad (2.1)$$

Eigenfunctions:

$$u_t = -2tL[u] + f(x, t)$$

where

$$L = \partial_{xx}, \quad f(x, t) = e^{-t^2} \sin x$$

Note that we cannot put t in the definition of L , since L must only involve derivatives in x . The eigenvalues/functions are

$$\lambda_n = n^2, \quad \phi_n(x) = \sin(nx), \quad n = 1, 2, \dots$$

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

because $\{e_k(t)\}_{k \in \mathbb{Z}} = \{e^{2i\pi kt}\}_{k \in \mathbb{Z}}$ is a Hilbert basis.

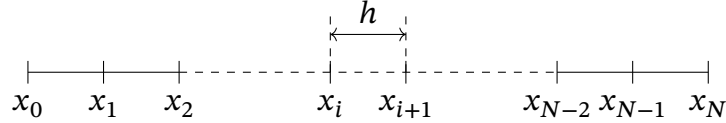


Figure 2: Equilong discretization in one dimension

The subsection [1.3](#) inspires us

$$\hat{f}(k) = \int_0^\tau f(x) e^{-2i\pi kx} dx \xrightarrow{\text{discretization}} U_k = \frac{1}{N} \sum_{j=0}^{N-1} f\left(\frac{j}{N}\right) e^{-2i\pi k \frac{j}{N}} \quad (2.2)$$

unequal lengths

2.1.1 FFT: interlacement

2.2 Finite Difference Method (FDM) for 1D Heat Equation

2.2.1 Explicit Euler's scheme

First, we determine the heat equation we need to consider

$$\begin{cases} \frac{\partial u}{\partial t}(x, t) + \frac{\partial^2 u}{\partial x^2}(x, t) = f(x, t), \\ u(x, 0) = u_0(x) \text{ in } \Omega, \\ u(0, t) = u(L, t) = g(t) \text{ on } (0, T), \end{cases} \quad (2.3)$$

The general idea of finite difference methods for evolution equations is that we replace the continuous variables in time and space with discrete points. In the case of an evolution equation, we need a spacetime grid. Let us thus be given two positive integers N and M . We set $h = \delta x = \frac{1}{N+1}$ and $X_n = nh$ for $n = 0, 1, 2, 3, \dots, N+1$. We set $k = \delta t = \frac{T}{M+1}$ and $t_j = jk$ for $j = 0, 1, 2, 3, \dots, M+1$. The parameter h is called the space grid step and the parameter k the time grid step, or time step. The grid points are the points (x_n, t_j) . We will let N and M go to infinity, or h and k go to 0.

The u_n^j for the above values of n and j , and it is hoped that u_n^j will be an approximation of $u(x_n, t_j)$, that should become better and better as N and M are increased. The boundary condition can be enforced exactly by requiring that

$$u_0^j = u_{N+1}^j = 0$$

And we note that $j = 0, 1, 2, 3, \dots, M + 1$. By the initial condition, we can acquire that

$$u_n^0 = u_0(x_n)$$

And we note that $n = 1, \dots, N$.

In this way, we will find that all the points of the boundary are known. The only values that are left unknown at this stage are thus u_n^j for $n = 1, 2, 3, \dots, N$ and $j = 1, 2, 3, \dots, M + 1$. We define that

$$U^j = \begin{pmatrix} u_1^j \\ u_2^j \\ \vdots \\ u_N^j \end{pmatrix} \in \mathbb{R}^N \quad (2.4)$$

Next, we need to calculate the remaining unknown points through the points of the known boundary. In the explicit Euler three point scheme, we can use the forward differential quotient approximation

$$\frac{\partial u}{\partial t}(x_n, t_j) \approx \frac{u(x_n, t_{j+1}) - u(x_n, t_j)}{k} \quad (2.5)$$

and for the second order space derivative, Using the same approximation, we can get:

$$\frac{\partial^2 u}{\partial x^2}(x_n, t_j) \approx \frac{\frac{u(x_{n+1}, t_j) - u(x_n, t_j)}{h} - \frac{u(x_n, t_j) - u(x_{n-1}, t_j)}{h}}{h} = \frac{u(x_{n+1}, t_j) - 2u(x_n, t_j) + u(x_{n-1}, t_j)}{h^2} \quad (2.6)$$

We substitute (3) and (4) into (1), we can get

$$\begin{cases} \frac{u_n^{j+1} - u_n^j}{k} - \frac{u_{n+1}^j - 2u_n^j + u_{n-1}^j}{h^2} = f_n^j \text{ for } n = 1, 2, 3, \dots, N, j = 0, 1, 2, 3, \dots, M, \\ u_n^0 = u_0(x_n) \text{ for } n = 1, \dots, N \\ u_0^j = u_{N+1}^j = 0 \text{ for } j = 0, \dots, M + 1 \end{cases} \quad (2.7)$$

So, we can rewrite the first N equations of the scheme in vector form as

$$\frac{U^{j+1} - U^j}{k} + A_h U^j = F^j \text{ for } j = 0, 1, 2, 3, \dots, M, \quad (2.8)$$

where A_h is the same $N \times N$ tridiagonal matrix

$$A_h = \begin{pmatrix} 2 & -1 & 0 & \dots & 0 \\ -1 & 2 & -1 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & -1 & 2 & -1 \\ 0 & \dots & 0 & -1 & 2 \end{pmatrix} \quad (2.9)$$

And we define that F_j and the discrete initial condition are two vectors of \mathbb{R}^N .

$$F^j = \begin{pmatrix} f_1^j \\ f_2^j \\ \vdots \\ f_N^j \end{pmatrix} \in \mathbb{R}^N \quad U_0 = \begin{pmatrix} u_0(x_1) \\ u_0(x_2) \\ \vdots \\ u_0(x_N) \end{pmatrix} \in \mathbb{R}^N \quad (2.10)$$

So, we can get the numerical scheme :

$$\begin{cases} U^{j+1} = (I - kA_h)U^j + kF^j \text{ for } j = 0, \dots, M \\ U^0 = U_0 \end{cases} \quad (2.11)$$

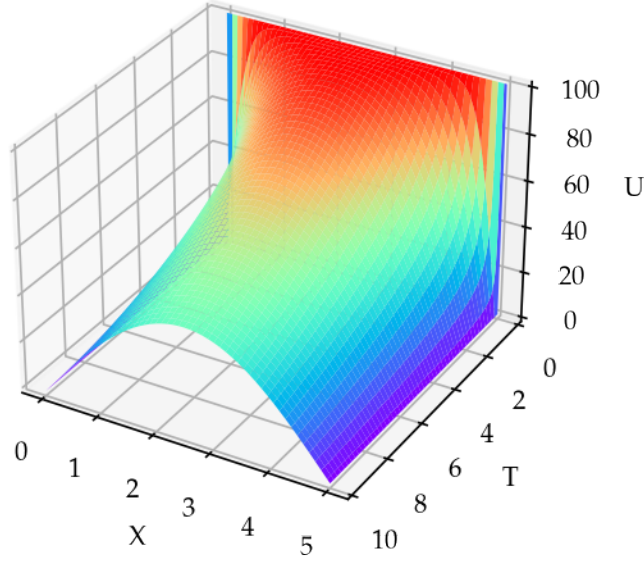


Figure 3: The numerical scheme for the 1D diffusion equation

2.2.2 Implicit Euler's scheme

2.2.3 Crank-Nicolson method

$$\begin{cases} \frac{u_i^{j+1} - u_i^j}{k} + \frac{1}{2} \left(-\frac{u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}}{h^2} + \frac{u_{i+1}^j - u_{i-1}^j}{h} \right) \\ + \frac{1}{2} \left(-\frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{h^2} + \frac{u_{i+1}^j - u_{i-1}^j}{h} \right) = \frac{1}{2}f(x_i, t_{j+1}) + \frac{1}{2}f(x_i, t_j), & i \in \{1, \dots, N\}, j \in \{1, \dots, J\} \\ u_i^0 = 0, & i \in \{1, \dots, N\} \\ u_0^j = u_{N+1}^j = 0, & j \in \{0, \dots, J\} \end{cases} \quad (2.12)$$

From 2.12, we could establish directly the relationship

$$\frac{1}{k}(U^{j+1} - U^j) + \frac{1}{2} \left(\frac{1}{h^2}AU^{j+1} + \frac{1}{h}BU^{j+1} \right) + \frac{1}{2} \left(\frac{1}{h^2}AU^j + \frac{1}{h}BU^j \right) = \frac{1}{2}(F^{j+1} + F^j) \quad (2.13)$$

with

$$A = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 & \dots & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & \dots & 0 \\ 0 & 0 & \dots & \dots & \dots & \dots & \dots & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & -1 & 2 \end{pmatrix} \quad B = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & \dots & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & \dots & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 & \dots & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & \dots & \dots & \dots & \dots & \dots & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & -1 & 0 \end{pmatrix} \quad (2.14)$$

We reformulate the method 2.12 in a condensed way:

$$\begin{cases} \left(I + \frac{k}{2}C\right) U^{j+1} = \left(I - \frac{k}{2}C\right) U^j + \frac{k}{2}(F^{j+1} + F^j), & j \in \{1, \dots, J\} \\ U^0 = 0 \end{cases} \quad (2.15)$$

then A, B, C satisfied $C = \frac{1}{h^2}A + \frac{1}{h}B$, we shall write C explicitly:

$$C = \frac{1}{h^2} \begin{pmatrix} 2 & -1+h & 0 & 0 & 0 & \dots & 0 \\ -1-h & 2 & -1+h & 0 & 0 & \dots & 0 \\ 0 & -1-h & 2 & -1+h & 0 & \dots & 0 \\ 0 & 0 & -1-h & 2 & -1+h & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & \dots & \dots & \dots & 0 & 2 & -1+h \end{pmatrix} \quad (2.16)$$

This vector form 2.15 is finally realize in Python:

```
1 def matrix_CF(N, func):
2     # N as the number of knots (INCLUDING END POINTS)
3     h = 1/(N-1)
4     h_coeff = h**(-2)
5
6     # Creation of diagonal part of C_h
7     vect0 = h_coeff*2 * np.ones(N)
8     C0 = np.diagflat(vect0, 0)
9
10    # upper part of C_h
11    vect1 = h_coeff*(-1+h) * np.ones(N-1)
12    C1 = np.diagflat(vect1, 1)
13
14    # lower part of C_h
15    vect2 = h_coeff*(-1-h)*np.ones(N-1)
16    C2 = np.diagflat(vect2, -1)
17
18    # assembly C_h
19    C_h = C0 + C1 + C2
20
21    x = np.linspace(0, 1, N)
22    F_h = func(x)
23
24    return C_h, F_h
```

Listing 1: Martix representation of C in python

Given $N, M \in \mathbb{N}^*$ the number of knots incluing end points, we take space step size $h = 1/(N - 1)$ and set inner point $x_i = ih$, similally temporal step size is set as $k = 1/(M - 1)$. The unknown values are $u_1^j, u_2^j, \dots, u_N^j$. For $i = 1, \dots, N$ et $j = 1, \dots, M+1$, the corresponding unknown vector is $U^j = (u_1^j, \dots, u_N^j)^T$. Because u_0^j, u_1^j are in $\partial]0, 1[$, which is not defined here.

At each mesh point establishes the approximation $u_i^j \approx u(x_i, t_j)$ where in our case, the null frontier permets us to write F^j as $(f_1^j, f_2^j, \dots, f_N^j)^T$.

It's recommended to use the sparse matrix to represent the matrix C , which could be implemented by `import scipy.sparse`. The core Python snippets to solve linear system 2.15 is

```

1 def FDM_CN(N, M, f):
2     h = 1/(N-1)
3     k = 1/(M-1)
4     t = np.linspace(0, 1, M)
5     x = np.linspace(0, 1, N)
6     U = np.zeros((N, M+1))
7     # U[:, 0] = u(x,0) = 0 already satisfied
8
9     C_h, F_h = matrix_CF(N, f)
10
11     U[:, 0] = N*[0]
12     U[0, :] = U[-1, :] = (M+1)*[0]
13     for j in range(M):
14         U[:, j+1] = np.linalg.solve(np.eye(N)+k/2*C_h,\
15                                     np.matmul((np.eye(N) - k/2*C_h), U[:, j]) + k*F_h)
16
17     return t, U

```

Listing 2: the Crank-Nicolson method for system linear system 2.15

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

✦ **Definition 3.1** (truncation error): *In a word, truncation error is an error caused by approximating a mathematical process.*

In Fourier analysis we have our classical truncation error (inducted from Bessel's inequality and Parseval's equality) defined by

$$\varepsilon_{\text{Fourier}}[M] = \|f - \tilde{f}_M\|^2 = \sum_{k > M/2} |\langle f(\xi), e^{2i\pi k \xi} \rangle|^2 \quad (3.1)$$

In general FDM,

$$\varepsilon_{\text{FDM}} = \varepsilon_{h,k}(u)^j = \sum_{i=-m}^l B_i S_h(u_{t_{j+i}}) + \tilde{F}_j, \quad m \leq j \leq (\frac{T}{k} - l) \quad (3.2)$$

✦ **Definition 3.2** (consistency):

For different methods, we shall develop a general frame to

✦ **Definition 3.3:** *We say that the scheme (?) is consistent for the family of norms $\|\cdot\|_N$ if*

$$\max_{m \leq j \leq (\frac{T}{k} - l)} \|\varepsilon_{h,k}(u)^j\|_N \xrightarrow{(h,k) \rightarrow (0,0)} 0 \quad (3.3)$$

And we say it's of order p in space and q in time for the family of norms $\|\cdot\|_N$ if

$$\max_{m \leq j \leq (\frac{T}{k}-1)} \left\| \varepsilon_{h,k}(u)^j \right\|_N \leq C_u(h^p + k^q) \quad (3.4)$$

Where C_u is a constant that depends only on u .

Consistency means that the scheme is trying its best to locally approximate the right numerical problem in the norm $\|\cdot\|_N$.

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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