AMSC/CMSC 661 Scientific Computing II
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Solution of Parabolic Partial Differential Equations
Part 1: Theory
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These notes are based on the 2003 textbook
of Stig Larsson and Vidar Thomée.

Parabolic equations, two problems

The Pure Initial Value Problem: when $x \in \mathcal{R}^d$.

$$\begin{aligned} \frac{\partial u(x,t)}{\partial t} - \Delta u(x,t) &= 0 \quad \text{for } x \in \mathcal{R}^d, t \in \mathcal{R}_+ \\ u(x,0) &= v(x) \quad \text{for } x \in \mathcal{R}^d \end{aligned}$$

The Initial Boundary Value Problem: $x \in \Omega \subseteq \mathcal{R}^d$, with Ω bounded.

$$\begin{aligned} \frac{\partial u(x,t)}{\partial t} - \Delta u(x,t) &= 0 \quad \text{for } x \in \Omega \subset \mathcal{R}^d, t \in \mathcal{R}_+ \\ u(x,0) &= v(x) \quad \text{for } x \in \Omega \\ u(x,t) &= 0 \quad \text{for } x \in \Gamma(\Omega), t \in \mathcal{R}_+ \end{aligned}$$

The differential equation in these problems is called the **heat equation**.

Note: parabolic equations are of the form $\partial u/\partial t$ **+ elliptic operator =** f.

Although we only consider the elliptic operator $-\Delta u$, more general ones can be used.

The Plan

- Some facts about the Fourier transform
- Solution of the pure IVP using the Fourier transform
- Solution of the Initial-Boundary Value Problem using eigenfunctions
- The weak (variational) formulation
- A maximum principle

Reference: Appendix A.3, Chapter 8.

Some facts about the Fourier transform

Given a function $v : \mathcal{R}^d \to \mathcal{R}$ (or $\to \mathcal{C}$), define its **Fourier transform** (FT) to be

$$\mathcal{F}v(\xi) = \hat{v}(\xi) = \int_{\mathcal{R}^d} v(x) e^{-ix\cdot\xi} dx,$$

and define the **inverse Fourier transform** (IFT)

$$\mathcal{F}^{-1}v(x) = \frac{\mathbf{1}}{(\mathbf{2}\pi)^{\mathbf{d}}} \int_{\mathcal{R}^d} v(\xi) e^{+ix\cdot\xi} d\xi.$$

Recall the space $L_1(\Omega)$ of functions v for which

$$\int_\Omega |v(x)| dx$$

is finite (p.233).

Important properties, assuming $v \in L_1(\mathcal{R}^d)$

- **Fourier inversion formula:** $\mathcal{F}^{-1}(\mathcal{F}v) = v$.
- **Parseval's formula:** $(v, w) = (2\pi)^{-d}(\hat{v}, \hat{w})$.
- **A norm relation:** $\|v\| = (2\pi)^{-d/2}\|\hat{v}\|$.
- **A translation relation:** if $w(x) = v(x + y)$ where y is fixed, then $\mathcal{F}w(\xi) = e^{iy\cdot\xi}\hat{v}(\xi)$
- **A scaling relation:** if $w(x) = v(ax)$ where $a > 0$ is a fixed scalar, then $\mathcal{F}w(\xi) = a^{-d}\hat{v}(a^{-1}\xi)$.
- **A convolution relation:** Define

  $$(v * w)(x) = \int_{\mathcal{R}} v(x - y) w(y) dy.$$

  Then $\mathcal{F}(v * w)(\xi) = \hat{v}(\xi)\hat{w}(\xi)$.

- (Most important for us right now) **A differentiation formula** that holds as long as v and its derivatives go to zero for large $|x|$:

  $$\mathcal{F}(D^\alpha v)(\xi) = i^{|\alpha|}\xi^\alpha \hat{v}(\xi)$$

  where $\xi^\alpha = \xi_1^{\alpha_1}\xi_2^{\alpha_2}\dots\xi_d^{\alpha_d}$.

  Example: $d = 3$:

  $$\mathcal{F}(u_{xxyzzz})(\xi) = (\sqrt{-\mathbf{1}})^{\mathbf{6}}\xi_1^2\xi_2\xi_3^3\hat{\mathbf{u}}(\xi)$$

  since $\alpha = (2, 1, 3)$.

Proofs of these properties (or at least sketches of them) can be found in Appendix A.3.

If you haven't seen this material before, it is worthwhile to

- Verify the properties for $d = 1$.
- Work though an example for $d = 1$.

An example verification

Let's verify a special case of the last one, letting $d = 1$ and $\alpha = 1$:

$$\mathcal{F}(D^\alpha v)(\xi) = i^{|\alpha|}\xi^\alpha \hat{v}(\xi).$$

Then, by Integration by Parts (our 2nd favorite calculus theorem):

$$\begin{array}{rcll} \hat{v'}(\xi) = & & \int_{-\infty}^{\infty} v'(x) e^{-ix\xi} dx & \text{definition of } \hat{v'} \\ & = & -\int_{-\infty}^{\infty} v(x)(-i\xi) e^{-ix\xi} dx & \text{integration by parts} \\ & = & (i\xi)\int_{-\infty}^{\infty} v(x) e^{-ix\xi} dx & \text{pulling out the constant} \\ & = & (i\xi)\hat{v}(\xi) & \text{definition of } \hat{v}. \end{array}$$

(The boundary term disappears by our assumption that $v' \to 0$ for large $|x|$.)

Solution of the pure IVP using the Fourier transform

Recall the problem:

$$\begin{aligned} \frac{\partial u(x,t)}{\partial t} - \Delta u(x,t) &= 0 \quad \text{for } x \in \mathcal{R}^d, t \in \mathcal{R}_+ \\ u(x,0) &= v(x) \quad \text{for } x \in \mathcal{R}^d \end{aligned}$$

We assume that u and its derivatives are small for large $|x|$.

We take the Fourier transform with respect to the variable x, obtaining a function $\hat{u}(\xi, t)$ that satisfies the equation

$$\begin{aligned} \hat{u}_t - i^2|\xi|^2\hat{u} &= 0, \\ \hat{u}(\xi, 0) &= \hat{v}(\xi) \text{ for } \xi \in \mathcal{R}^d \end{aligned}$$

For each fixed value of ξ, this is an ODE, and we can write down its solution:

$$\hat{u}(\xi, t) = \hat{v}(\xi) e^{-t|\xi|^2}$$

But what is u?

- **Fact 1**: If $w = e^{-|x|^2}$, then $\hat{w} = \pi^{d/2} e^{-|\xi|^2/4}$.
  Therefore, since t is a constant in the Fourier transform, the scaling relation tells us that $e^{-t|\xi|^2}$ is the Fourier transform of
  $$U(x,t) = (4\pi t)^{-d/2} e^{-|x|^2/(4t)}.$$
- **Fact 2:** Recall that $\mathcal{F}(v * w)(\xi) = \hat{v}(\xi)\hat{w}(\xi)$.
  Therefore, $u = U * v$, so
  $$u(x,t) = (U * v)(x,t) = (4\pi t)^{-d/2} \int_{\mathcal{R}^d} v(y) e^{-|x-y|^2/(4t)} dy.$$

It is not so obvious that this u satisfies the initial conditions given for $t = 0$, since we divide by t twice, but if we take the limit as $t \to 0$, it all works, as long as v is bounded and continuous; see **Theorem 8.1** for the verification.
Therefore, we know that the solution exists.

Just as in our study of elliptic equations, we want to show that the problem is **well-posed**: that the solution exists, is unique, and is stable (small changes in the data make small changes in the solution).

Since the exponential function is positive,
$$|u(x,t)| \le (4\pi t)^{-d/2} \int_{\mathcal{R}^d} e^{-|x-y|^2/(4t)} dy \|v\|_{\mathcal{C}} = \|v\|_{\mathcal{C}},$$
so, for $t > 0$,
$$\|u(\cdot,t)\|_{\mathcal{C}} \le \|v\|_{\mathcal{C}}$$
and this establishes **stability**.

For **uniqueness**, assume that u_1 and u_2 both solve the differential equation with the same initial conditions. Then $w = u_1 - u_2$ solves the differential equation with initial conditions $w(x,0) = 0$. Therefore, stability says that $w = 0$, so $u_1 = u_2$.

Therefore, the problem is well-posed.

A curious problem: the backward heat equation (p112)

Let's change the sign in the differential equation:
$$\begin{aligned} \frac{\partial u(x,t)}{\partial t} + \Delta u(x,t) &= 0 \quad \text{for } x \in \mathcal{R}^d, t \in \mathcal{R}_+ \\ u(x,0) &= v(x) \quad \text{for } x \in \mathcal{R}^d \end{aligned}$$
The differential equation is called the **backward heat equation**.

For example, if $d = 1$ and $v(x) = n^{-1}\sin(nx)$ where n is a positive integer, then the solution is
$$u(x,t) = n^{-1} e^{n^2 t} \sin(nx),$$
verified by substituting it into the equation.

- $\|v\|_{\mathcal{C}} = n^{-1}$ ($\to 0$ as $n \to \infty$)
- $\|u(t)\|_{\mathcal{C}} = n^{-1} e^{n^2 t}$ ($\to \infty$ as $n \to \infty$)

This problem is **ill-posed**!

In other words, given a temperature distribution now, finding a temperature distribution at a later time is **well-posed**. But finding the temperature distribution at an **earlier time** is **ill-posed**.

A curious property (p113)

If we look at our representation of the solution to the heat equation

$$u(x,t) = (U * v)(x,t) = (4\pi t)^{-\mathbf{d/2}} \int_{\mathcal{R}^d} v(y) e^{-|x-y|^2/(4t)} dy.$$

we can convince ourselves that we can compute any partial derivative of u that we desire – they all exist, **even if v is not smooth**.

If v **is** smooth, then the derivatives exist and are bounded uniformly for $t > 0$.

Adding a forcing function (p113)

$$\begin{aligned} \frac{\partial u(x,t)}{\partial t} - \Delta u(x,t) &= \mathbf{f} && \text{for } x \in \mathcal{R}^d, t \in \mathcal{R}_+ \\ u(x,0) &= v(x) && \text{for } x \in \mathcal{R}^d \end{aligned}$$

has the solution

$$\begin{aligned} u(x,t) &= (4\pi t)^{-d/2} \int_{\mathcal{R}^d} v(y) e^{-|x-y|^2/(4t)} dy \\ &\quad + (4\pi t)^{-d/2} \int_0^t \int_{\mathcal{R}^d} f(y,s) e^{-|x-y|^2/(4(t-s))} dy\, ds. \end{aligned}$$

if v, f, and $\bigtriangledown f$ are continuous and bounded.

Solution of the IBVP using eigenfunctions

Warning: In Section 8.2 of the text, i is just an index (not $\sqrt{-1}$) and $\hat{u}$ is just a function (not the Fourier transform). This can be confusing, so I'll avoid i's and $\hat{}$ in these notes by changing notation.

The previous technique is great for determining temperature of infinite bodies. Let's move on to finite ones.

$$\begin{aligned} \frac{\partial u(x,t)}{\partial t} - \Delta u(x,t) &= 0 && \text{for } x \in \Omega \subset \mathcal{R}^d, t \in \mathcal{R}_+ \\ u(x,0) &= v(x) && \text{for } x \in \Omega \\ u(x,t) &= 0 && \text{for } x \in \Gamma(\Omega), t \in \mathcal{R}_+ \end{aligned}$$

Note that we now need **boundary conditions** in addition to our initial conditions.

Let's pull out our complete set of orthonormal eigenfunctions for $-\Delta u = \lambda u$ on Ω. Call the eigenvalues $0 < \lambda_1 \leq \lambda_2 \leq \ldots$ and call the eigenfunctions z_j, **so that $-\Delta z_j = \lambda_j z_j$ and $z_j = 0$ on Γ.**

We'll **separate variables** and try to express u as a sum of z's:

$$u(x,t) = \sum_{j=1}^{\infty} \mathbf{w_j(t)} z_j(x)$$

and see if we can find functions $w_j(t)$ to make this work.

Note that the **boundary conditions** are automatically satisfied.

Let's try to **satisfy the PDE**:

$$\begin{aligned} u_t &= \sum_{j=1}^{\infty} w_j'(t) z_j(x) \\ -\Delta u &= \sum_{j=1}^{\infty} w_j(t) \lambda_{\mathbf{j}} z_j(x) \end{aligned}$$

so

$$u_t - \Delta u = \sum_{j=1}^{\infty} (w_j'(t) + \lambda_{\mathbf{j}} w_j(t)) z_j(x) = 0.$$

Since the z_j form a basis, we must have

$$w_j' + \lambda_{\mathbf{j}} w_j = 0$$

for $t > 0$, and we know the solution to ODEs that look like this:

$$w_j(t) = w_j(0) e^{-\lambda_{\mathbf{j}} t}.$$

Finally, in order to satisfy the **initial conditions** we set

$$u(x,0) = \sum_{j=1}^{\infty} w_j(0) z_j(x) = v(x),$$

so

$$w_j(0) = (v, z_j) = \int_{\Omega} v(x) z_j(x) dx.$$

So the solution to our IBVP is

$$u(x,t) = \sum_{j=1}^{\infty} w_j(0) e^{-\lambda_{\mathbf{j}} t} z_j(x)$$

Example: See top of p. 118.

Properties of the solution

$$u(x,t) = \sum_{j=1}^{\infty} (v, z_j) e^{-\lambda_j t} z_j(x)$$

- (p115)

$$\|u(\cdot,t)\|^2 \le e^{-2\lambda_1 t} \sum_{j=1}^{\infty} (v, z_j)^2 \le e^{-2\lambda_1 t} \|v\|^2$$

  and this is finite. (The last inequality comes from Parseval's relation, and the norm is L_2.)

- (p115) $u(x,t)$ is **smooth** for $t > 0$ (since we can differentiate our formula as much as we want).
- We could add a right-hand side function f as before; see p. 118 for details.

The weak(variational) formulation

- Take the PDE: $u_t - \Delta u = f$.
- Take the inner product with an arbitrary function $\phi \in H_0^1$:

$$(u_t, \phi) + a(u, \phi) = (f, \phi)$$

Weak formulation: Find $u \in H_0^1$ so that

$$(u_t, \phi) + a(u, \phi) = (f, \phi)$$

and $u(x,0) = v(x)$ for $x \in \Omega$.

As before, we can reverse the argument if u is smooth enough, so a smooth solution to the weak problem solves the strong problem.

Theorem 8.5 gives some bounds on the solution, proved by using the weak formulation.

Our main interest in the weak formulation, as before, is in using it as the basis for the finite element method.

A maximum principle

In practice, we only solve the problem for a **finite time interval** $[0, T]$. Define the **parabolic boundary** to be the set of (x,t) values where either

- $t = 0$ and $x \in \bar{\Omega}$, or
- $0 < t \leq T$ and $x \in \Gamma(\Omega)$.

We obtain two results that look like our results for elliptic equations and are proved similarly:

The maximum principle (Theorem 8.6). If u is smooth and $u_t - \Delta u \leq 0$ on $\Omega \times (\mathbf{0}, \mathbf{T})$, then u attains its maximum on the parabolic boundary.

A stability estimate (Theorem 8.7).

$$\|u\|_{\mathcal{C}(\bar{\Omega}\times[0,T])} \leq \max(\|g\|_{\mathcal{C}(\Gamma\times[0,T])}, \|v\|_{\mathcal{C}(\bar{\Omega})}) + \frac{r^2}{2d}\|f\|_{\mathcal{C}(\bar{\Omega}\times[0,T])}$$

where Ω is contained in a ball of radius r and $u = g$ **on** $\Gamma \times (0, T)$.