

PDEs, part 2: Parabolic PDEs

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Parabolic equations

(Sections 6.1, 6.2 and 6.5 of Strang).

Consider the model problem:

$$u_t = u_{xx} \quad x \in (0, 1), t > 0$$

$$u(x, 0) = g(x)$$

$$u(0, t) = u(1, t) = 0 \quad t > 0$$

t is time, x is the spatial variable. $u(x, t)$ can for example be the temperature in a rod with the initial temperature profile $g(x)$ at $t = 0$, whose ends are held at the temperature 0.
For well posedness, we need that:

- 1.** A solution exists.
 - 2.** The solution is unique.
 - 3.** The solution depend continuously on the data.
- We can show (1) by separation of variables.
For (2) and (3), we use the *Energy method*.

Diffusion on the whole line

Consider:

$$u_t = ku_{xx} \quad -\infty < x < \infty, t > 0$$

When considering the diffusion or heat equation on the whole line, we have five basic *invariance properties* of the diffusion equation :

1. The translate $u(x - y, t)$ of any solution $u(x, t)$ is another solution, for any fixed y .
2. Any derivative (u_x or u_t or u_{xx} etc) of a solution is again a solution.
3. A *linear combination* of solutions is again a solution.
4. An *integral* of solutions is again a solution. If $S(x, t)$ is a solution, so is $S(x - y, t)$ and so is

$$v(x, t) = \int_{-\infty}^{\infty} S(x - y, t) g(y) dy$$

for any function $g(y)$, as long as this improper integral converges.

5. If $u(x, t)$ is a solution, so is the *dilated* function $u(\sqrt{ax}, at)$.
(Show this by the chain rule).



The "diffusion kernel"

Using these properties, and some additional machinery, one can show that the solution to:

$$\begin{aligned} u_t &= ku_{xx} & -\infty < x < \infty, t > 0 \\ u(x, 0) &= g(x) \end{aligned}$$

can be written

$$u(x, t) = \int_{-\infty}^{\infty} S(x - y, t) g(y) dy, \quad \text{for } t > 0.$$

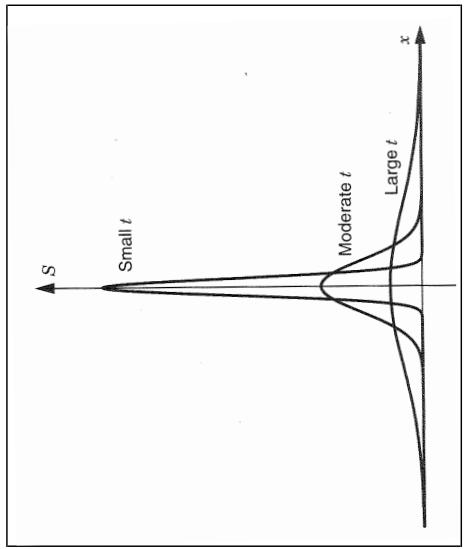
where

$$S(x, t) = \frac{1}{2\sqrt{\pi kt}} e^{-x^2/4kt}.$$

$S(x, t)$ is known as the fundamental solution, or free space Green's function, or the heat kernel or diffusion kernel.



The "diffusion kernel"



At all times, the area under its graph is:

$$\int_{-\infty}^{\infty} S(x, t) dx = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-q^2} dq = 1,$$

by substituting $q = x/\sqrt{4kt}$.

$S(x, t)$ is defined for all real x and for $t > 0$.

$$S(x, t) = \frac{1}{2\sqrt{\pi kt}} e^{-x^2/4kt}.$$

Initially, it is a tall spike. With time, it spreads and flattens out.

Numerical methods for the diffusion equation

We want to solve:

$$\begin{aligned} u_t &= u_{xx} & x \in (0, 1), t > 0 \\ u(x, 0) &= g(x) & (*) \\ u(0, t) &= u(1, t) = 0 & t > 0 \end{aligned}$$

Semi-discretization: The simplest way to derive useful numerical methods for (*) is to discretize only in space, to obtain a system of ODEs, and then apply an ODE solver to the problem.
Introduce

$$x_j = j\Delta x, \quad j = 0, \dots, N + 1, \quad \Delta x = \frac{1}{N + 1}$$

and let $u_j(t) \approx u(x_j, t)$.

Approximate the spatial derivative with for example central differences:

$$u_{xx}(x_j, t) \approx \frac{u_{j-1}(t) - 2u_j(t) + u_{j+1}(t)}{(\Delta x)^2}$$

Semi-discrete form

This yields the semi-discrete form of (*):

$$\frac{du_j(t)}{dt} = \frac{u_{j-1}(t) - 2u_j(t) + u_{j+1}(t)}{(\Delta x)^2}, \quad j = 1, \dots, N$$
$$u_j(0) = g(x_j) \quad (**)$$
$$u_0(t) = u_{N+1}(t) = 0$$

On matrix form, with $\mathbf{u} = (u_1, \dots, u_N)^T$ and $\mathbf{u}(0) = (g(x_1), \dots, g(x_N))^T$,

$$\frac{d\mathbf{u}}{dt} = \mathbf{A}\mathbf{u}.$$

Here,

$$\mathbf{A} = \frac{1}{(\Delta x)^2} \begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix} \in \mathbb{R}^{N \times N}.$$

Semi-discrete form → Method of lines

We have a PDE that we discretize in space to obtain a large system of ODEs. In this example, a central finite difference approximation.

Can also get a system of ODEs from a finite element discretization.

The problem (*) can now be discretized with a regular ODE solver, e.g forward Euler:

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t \mathbf{A}\mathbf{u}^n.$$

This approach is sometimes called *method of lines*, since one solves the problem along a set of lines, $x = \text{const}$, $t > 0$.

Linear Stability

A necessary condition for this to work is that the ODE method is linearly stable, i.e that

$$\Delta t \lambda_n \in D \quad \forall n,$$

where λ_n are the eigenvalues of \mathbf{A} and D is the linear stability region.

CFL condition

For our discretization (**) with forward Euler , the linear stability yields the restriction:

$$\mu := \frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{2}.$$

- When Δx is decreased, the size of \mathbf{A} increases, and we are solving different ODE systems. The linear stability depends on both Δt and Δx .
- μ is the so called *CFL number* (for Courant-Friedrichs-Lowy) or simply the Courant number. The condition is called a "CFL-condition".
- The condition $\Delta t < C(\Delta x)^2$ is typical for explicit time discretizations for parabolic problems. One therefore often prefers to use implicit methods.

Convergence?

- The ODE theory can only be used to prove convergence as $\Delta t \rightarrow 0$ with Δx fixed, and in that case only to the solution of the semi-discrete approximation.
- We need convergence as $\Delta t \rightarrow 0$ and $\Delta x \rightarrow 0$ simultaneously!
- Usually we have a fixed relation $\Delta t = \mu \Delta x^2$ or $\Delta t = \mu \Delta x$, and let $\Delta x \rightarrow 0$. To be able to analyze this convergence, we need to study a full discretization (FD) in time and space of (*).

Analysis

Let $\tilde{\mathbf{u}}^n = (\tilde{u}_1^n, \dots, \tilde{u}_N^n)^T$, where $\tilde{u}_j^n = u(x_j, t_n)$, the exact solution.

The solution of the discretized problem is $\mathbf{u}^n = (u_1^n, \dots, u_N^n)^T$.

Define the discrete L_2 -norm:

$$\|g\|_{\Delta x} = \left(\Delta x \sum g_j^2 \right)^{1/2}$$

The numerical solution converges to the true solution if

$$\lim_{\Delta x \rightarrow 0} \max_{0 \leq n \leq N_{\Delta t}} \|\mathbf{u}^n - \tilde{\mathbf{u}}^n\|_{\Delta x} = 0$$

when $\Delta t = \mu(\Delta x)^\alpha$ (for some μ, α), and $T = N_{\Delta t} \cdot \Delta t$ is fixed.

Usually, very difficult to prove convergence directly.

Luckily, we have a very powerful theorem to help us.

Lax equivalence theorem

The Lax equivalence theorem holds for a general linear well-posed time dependent PDE. For a finite difference method for such a problem it holds:

The method is convergent if it is *consistent* and *stable*.

or said differently:

A *consistent* method is *convergent if and only if it is stable*.

The Lax equivalence theorem is the fundamental theorem in the analysis of finite difference methods.

Consistency and stability

Consistent approximation

- Local truncation error: τ_j^n . Residual when inserting the exact solution \tilde{u}_j^n into the numerical scheme.
- If $\tau_j^n = O((\Delta x)^p + (\Delta t)^q)$ we say that the method is of order p in space and q in time.
- The method is consistent if $p \geq 1$ and $q \geq 1$.

Stability

- We say that the method is stable if

$$\|\mathbf{u}^n\|_{\Delta x} \leq C(T) \|\mathbf{u}^0\|_{\Delta x} \quad \text{for } n = 0, \dots, N_{\Delta t},$$

where $N_{\Delta t} \cdot \Delta t = T$ and $\Delta t = \mu(\Delta x)^\alpha$ (for some μ, α).

- OBS! $C(T)$ does not depend on Δt or Δx .

Examples of discretizations

- Euler's method (Forward Euler + central differences).
- Crank-Nicolson (Trapezoidal rule + central differences).

[NOTES]

Both these discretizations are so called one-step methods. To evaluate on level $n+1$, only values at level $n+1$ and n , one level back, are used. The general formula for a one-step method is

$$\sum_{k=-\gamma}^{\delta} b_k(\mu) u_{j+k}^{n+1} = \sum_{k=-\alpha}^{\beta} c_k(\mu) u_{j+k}^n,$$

(together with boundary conditions), where $\mu = (\Delta t)/(\Delta x)^2$. With this way of writing it, τ_j^n is defined by

$$\tau_j^n = \frac{1}{\Delta t} \left(\sum_{k=-\gamma}^{\delta} b_k(\mu) \tilde{u}_{j+k}^{n+1} - \sum_{k=-\alpha}^{\beta} c_k(\mu) \tilde{u}_{j+k}^n \right),$$

where $\tilde{u}_j^n = u(x_j, t_n)$ is the exact solution.

Fourier analysis, continuous problem.

Consider the Cauchy problem ($-\infty < x < \infty$),

$$u_t = ku_{xx}, \quad u(x, 0) = f(x).$$

Assume $f(x)$ on the form $f(x) = e^{i\omega x} \hat{f}(\omega)$.
Look for solutions of the same type, $u(x, t) = e^{i\omega x} \hat{u}(\omega, t)$.

This yields "the Fourier transform of the equation"

$$\hat{u}_t = -\omega^2 \hat{u}, \quad \hat{u}(\omega, 0) = \hat{f}(\omega).$$

We have, $\hat{u}(\omega, t) = e^{-\omega^2 t} \hat{u}(\omega, 0) = e^{-\omega^2 t} \hat{f}(\omega)$, and so

$$u(x, t) = e^{i\omega x} e^{-\omega^2 t} \hat{f}(\omega).$$

Fourier analysis, continuous problem, continued

Now, consider the general case: $f(x) = \sum_{\omega=-\infty}^{\infty} e^{i\omega x} \hat{f}(\omega)$.

By superposition:

$$u(x, t) = \sum_{\omega=-\infty}^{\infty} e^{i\omega x} e^{-\omega^2 t} \hat{f}(\omega).$$

For every fixed t , Parseval's relation yields

$$\|u(\cdot, t)\|^2 = 2\pi \sum_{\omega=-\infty}^{\infty} |e^{i\omega x} e^{-\omega^2 t} \hat{f}(\omega)|^2 \leq 2\pi \sum_{\omega=-\infty}^{\infty} |\hat{f}(\omega)|^2 = \|f(\cdot, t)\|^2,$$

for the L_2 -norm,

$$\|g\| = \left(\int_0^{2\pi} g(x)^2 dx \right)^{1/2}.$$

(f and u 2π -periodic functions).

Fourier analysis, discrete problem

Assume $f_j = e^{i\omega x_j} \hat{f}(\omega)$.

Look for solutions, $u_j^n = \hat{u}^n(\omega) e^{i\omega x_j}$.

Consider the discrete one step method:

$$\sum_{k=-\gamma}^{\delta} b_k(\mu) u_{j+k}^{n+1} = \sum_{k=-\alpha}^{\beta} c_k(\mu) u_{j+k}^n.$$

Plug in the solution,

$$\sum_{k=-\gamma}^{\delta} b_k(\mu) \hat{u}^{n+1} e^{i\omega(x_j + \Delta x k)} = \sum_{k=-\alpha}^{\beta} c_k(\mu) \hat{u}^n e^{i\omega(x_j + \Delta x k)}$$

and so

$$\hat{u}^{n+1}(\omega) = \hat{Q}(\omega) \hat{u}^n(\omega), \quad \text{or} \quad \hat{u}^n(\omega) = (\hat{Q}(\omega))^n \hat{f}(\omega),$$

where

$$\hat{Q}(\omega) = \frac{\sum_{k=-\alpha}^{\beta} c_k(\mu) e^{i\omega(k \Delta x)}}{\sum_{k=-\gamma}^{\delta} b_k(\mu) e^{i\omega(k \Delta x)}}$$



Fourier analysis, discrete problem

$\hat{Q}(\omega)$ is the growth factor, or amplification factor.

It shows how each frequency ω is amplified.

We say that the method is stable if

$$\|\mathbf{u}^n\|_{\Delta x} \leq C(T) \|\mathbf{u}^0\|_{\Delta x} \quad \text{for } n = 0, \dots, N_{\Delta t},$$

where $N_{\Delta t} \cdot \Delta t = T$ and $\Delta t = \mu(\Delta x)^\alpha$ (for some μ, α).

OBS! $C(T)$ does not depend on Δt or Δx .

For this to be true, for each frequency ω , we need

$$\hat{Q}(\omega) \leq 1 + C \cdot \Delta t.$$

This is the so called von Neumann analysis.

The condition based on von Neumann analysis guarantees stability in this case. This is true for all linear PDEs with constant coefficients and periodic boundary conditions / problems on the whole line.

The analysis yields a *necessary* condition for a much wider class of problems, but is then not sufficient to guarantee stability.

