

Partial Differential Equations, lecture 4

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Maximum Principle

The fact that the heat flows from higher to lower temperatures implies that the solution of the homogeneous heat equation attains its maximum and minimum values on $\partial Q_T = \overline{Q_T} - Q_T$. The following result known as the [maximum principle](#) summarizes this idea. Before we give the statement of the theorem, let us introduce some notation. It is occasionally useful to consider spaces of functions with different smoothness in the x and t variables. We will use $C^{2,1}(Q_T)$ to denote the space of functions with continuous first and second order derivatives in space and continuous derivatives in time. I.e.

$$C^{2,1}(Q_T) = \{u : Q_T \rightarrow \mathbb{R} \mid u, D_x u, D_x^2 u, u_t \in C(Q_T)\} \quad (1)$$

From this, we can state our maximum principle

Theorem 1 (Maximum Principle). *Assume $u \in C^{2,1}(Q_T) \cap C(\overline{Q_T})$ solves the heat equation in Q_T*

(i) *then*

$$\begin{cases} \max_{\overline{Q_T}} u = \max_{\partial Q_T} u \\ \min_{\overline{Q_T}} u = \min_{\partial Q_T} u \end{cases} \quad (2)$$

(ii) *Furthermore, if U is connected and there exists a point $(x_0, t_0) \in Q_T$ such that*

$$u(x_0, t_0) = \max_{\overline{Q_T}} u \quad (3)$$

then u is constant in $\overline{Q_{t_0}}$

The first part of Theorem 1 (which we are going to prove) is known as the [weak maximum principle](#). Part (ii) is known as the [strong maximum principle](#).

Proof. To prove part (i), we will start by showing that the statement holds for a function v for which the heat equation takes a negative value. We will then use this result for $\epsilon \rightarrow 0$ to derive the result on any solution $u(x, t)$ of the heat equation.

Let $u(x, t) \in C^{2,1}(Q_T) \cap C(\bar{Q}_T)$ satisfy the equation

$$\frac{\partial u}{\partial t} - D\Delta u = 0 \quad (4)$$

Let us define $v(x, t)$ as $v(x, t) = u(x, t) - \epsilon t$ for $\epsilon > 0$. Note that this definition in particular implies

$$\frac{\partial v}{\partial t} - D\Delta v = -\epsilon + \frac{\partial u}{\partial t} - D\Delta u = -\epsilon < 0 \quad (5)$$

We will first show that for $v(x, t)$,

$$\max_{\bar{Q}_T} v = \max_{\partial Q_T} v \quad (6)$$

to see this, let us use contradiction and assume that there exists $(x_0, t_0) \in Q_T$ such that (x_0, t_0) is a maximum of v (that is to say such that $\max_{\bar{Q}_T} v = v(x_0, t_0)$). Recall that

- 1) For $v(x, t) : Q_T \rightarrow \mathbb{R}$ defined on the set $Q_T \subseteq \mathbb{R}^n$, if $(x_0, t_0) \in Q_T$ is a local optimum point and all the partial derivatives of v exist at (x_0, t_0) , then $\nabla v(x_0, t_0) = 0$
- 2) For $v(x, t) : Q_T \rightarrow \mathbb{R}$ defined on an open set $Q_T \subseteq \mathbb{R}^n$, if $v(x, t)$ is twice continuously differentiable over Q_T and if (x_0, t_0) is a stationary point, then if (x_0, t_0) is a local maximum of v , $\nabla^2 v(x_0, t_0) \preceq 0$.

From those two conditions, we see that if (x_0, t_0) is a local maximum of $v(x, t)$ on Q_T , we necessarily have $v_{x_i x_i}(x_0, t_0) \leq 0$ (this is implied by the negative semidefiniteness of the Hessian¹). Moreover, since x_0 is in Q_T which is an open set (except at $t = T$), we must have $v_x(x_0, t_0) = 0$. For the time variable, this is a little different. As the set includes the $t = T$ line, we cannot guarantee that the maximum lies within an open ball and the best we can say is that $v_t(x_0, t_0) \geq 0$. Indeed, if we take any $h > 0$, as (x_0, t_0) is a maximum on \bar{Q}_T , we always have

$$\frac{v(x_0, t_0) - v(x_0, t_0 - h)}{h} \geq 0$$

and hence

$$\lim_{h \rightarrow 0} \frac{v(x_0, t_0) - v(x_0, t_0 - h)}{h} = v_t(x_0, t_0) \geq 0$$

¹Negative semidefinite matrices have all their diagonal entries that are non positive. In this case the diagonal entries of $\nabla^2 v(x_0, t_0)$ are precisely the derivatives $\partial_{x_i x_i} v(x_0, t_0)$

Grouping our conditions on the space and time derivatives, and substituting in the heat equation, we get

$$v_t(x_0, t_0) - D\Delta v(x_0, t_0) \geq 0 \quad (7)$$

which is in contradiction with (5). We can thus assume that (6) holds, that is, $v(x, t)$ achieves its maximum on ∂Q_T .

Now from the definition of u , we have

$$\max_{\overline{Q_T}} v(x, t) = \max_{\partial Q_T} v(x, t) \leq \max_{\partial Q_T} u(x, t) \quad (8)$$

Taking the limit as $\varepsilon \rightarrow 0$, we get

$$\lim_{\varepsilon \rightarrow 0} \max_{\overline{Q_T}} u(x, t) - \varepsilon t \leq \max_{\partial Q_T} u(x, t) \quad (9)$$

which implies

$$\max_{\overline{Q_T}} u(x, t) \leq \max_{\partial Q_T} u(x, t) \quad (10)$$

□

Invariant transformations, similarities, and Fundamental solution

Although the solution of the homogeneous heat equation is non unique, there are privileged solutions which can be used to create many others. To introduce those solutions, we will start by discussing invariant transformations.

The homogeneous heat equation has simple but important properties. Let $u = u(x, t)$ be a solution of the diffusion equation

$$u_t - D\Delta u = 0 \quad (11)$$

Obviously the function $v(x, t) = u(x, -t)$ obtained by the change of variables $t \mapsto -t$ is a solution of the adjoint or backward equation

$$v_t + D\Delta v = 0 \quad (12)$$

Two other important invariant transformations are space and time translations as well as parabolic dilations

- **Space and time translations.** For y, s fixed, the function $v(x, t) = u(x - y, t - s)$ is still a solution of (11).

- **Parabolic dilations.** The transformation

$$x \mapsto ax, \quad t \mapsto bt, \quad u \mapsto cu, \quad (a, b, c > 0) \quad (13)$$

represents a dilation (expansion or contraction) of the graph of u . Let us check for which values of a, b, c the function

$$u^*(x, t) = cu(ax, bt) \quad (14)$$

is still a solution of (11). We have

$$u_t^*(x, t) - D\Delta u^*(x, t) = cbu_t(ax, bt) - ca^2 D\Delta u(ax, bt)$$

and so u^* is a solution of (11) if $b = a^2$. The relation above suggests the name of parabolic dilations for the transformation

$$x \mapsto ax, \quad t \mapsto a^2t, \quad (a, b > 0).$$

In particular note that under those transformations, the ratios

$$\frac{|x|^2}{Dt}, \frac{|x|^2}{t}, \quad \text{as well as} \quad \frac{x}{\sqrt{Dt}}, \frac{x}{\sqrt{t}}, \quad \text{are left unchanged}$$

the first ratios $|x|^2/(Dt)$ and x/\sqrt{Dt} are especially interesting as they correspond (as we saw earlier) to dimensionless quantities.

Dilation and conservation of mass/energy

An other important property, when discussing the evolution of a density, or the evolution of temperature, is the conservation of mass/energy. If u is a solution of the heat equation, and in light of what was said above, one can wonder what are the transformations (e.g. dilations) that still satisfy this property. Suppose that $u(x, t)$ satisfies the relation

$$\int_{\mathbb{R}^n} u(x, t) dx = q, \quad \text{for every } t > 0$$

Letting $u^*(x, t)$ to denote the dilation $u^*(x, t) = cu(ax, a^2t)$, we get

$$\int_{\mathbb{R}^n} u^*(x, t) dx = c \int_{\mathbb{R}^n} u(ax, a^2t) dx = q.$$

Letting $y_i = ax_i$, we thus have $a^n dx = dy$ and hence

$$\int_{\mathbb{R}^n} u^*(x, t) dx = \frac{c}{a^n} \int_{\mathbb{R}^n} u(y, a^2t) dy$$

We see from this last relation that for u and u^* to satisfy the conservation of energy/mass (for a same fixed total energy q), we need $c/a^n = 1$.

In conclusion, if $u(x, t)$ is a solution to the heat equation that satisfies the conservation of mass (with total mass q), so does any solution of the form

$$u^*(x, t) = a^n u(ax, a^2t)$$

Given the invariances we unveiled, a natural approach would be to wonder if those invariances do not simply arise from the particular structure of the solution. I.e. maybe what we assumed to be different solutions are just a single solution defined as a function of our invariants. In other words, if it seems that any solution of the form $a^n u(ax, a^2 t)$ is a solution, perhaps it is because the solutions have the form

$$U\left(\frac{|x|^2}{Dt}\right), \quad \text{or} \quad U\left(\frac{|x|^2}{t}\right)$$

for some appropriate function U . It therefore seems like a reasonable idea to look for solutions of this form. Such solutions, called similarity solutions, would explain the invariance as

$$u(\lambda x, \lambda^2 t) = U\left(\frac{\lambda^2 |x|^2}{\lambda^2 t}\right) = U\left(\frac{|x|^2}{t}\right) = u(x, t)$$

and similarly for $U\left(\frac{|x|}{\sqrt{Dt}}\right)$.

As in the general case, note that for such solutions to satisfy the conservation of mass, we must have

$$\begin{aligned} q &= \int_{\mathbb{R}^n} U\left(\frac{|x|}{\sqrt{Dt}}\right) dx \\ &= \int_{\mathbb{R}^n} U\left(\frac{|x|}{\sqrt{\lambda Dt}}\right) dx, \quad \text{for any } \lambda \in \mathbb{R}^+ \\ &= \int_{\mathbb{R}^n} U\left(\frac{\sqrt{\sum_{i=1}^n \left(\frac{x_i^2}{\lambda^{1/2}}\right)}}{\sqrt{Dt}}\right) \frac{dx_1}{\lambda^{1/2}} \cdots \frac{dx_n}{\lambda^{1/2}} \lambda^{n/2} dx \\ &= \lambda^{n/2} \int_{\mathbb{R}^n} U\left(\frac{|y|}{\sqrt{Dt}}\right) dy = \lambda^{n/2} \end{aligned}$$

Hence to cancel the $\lambda^{n/2}$, we might want to multiply our ansatz with $\frac{1}{(Dt)^{n/2}}$. From this, we get

$$\begin{aligned} \int_{\mathbb{R}^n} \frac{1}{(Dt)^{n/2}} U\left(\frac{|x|}{\sqrt{Dt}}\right) dx = q \quad \Rightarrow \quad \forall \lambda > 0, \quad \int_{\mathbb{R}^n} \frac{1}{(Dt)^{n/2}} \frac{1}{\lambda^{n/2}} U\left(\frac{|x|}{\sqrt{\lambda Dt}}\right) dx \\ = \int_{\mathbb{R}^n} \frac{1}{(Dt)^{n/2}} U\left(\frac{|y|}{\sqrt{Dt}}\right) dy = q \end{aligned}$$

Fundamental solution

We therefore look for solutions of the form

$$u^*(x, t) = \frac{1}{(Dt)^{n/2}} U\left(\frac{|x|}{\sqrt{Dt}}\right) \tag{15}$$

for which we require

$$\int_{\mathbb{R}^n} \frac{1}{(Dt)^{n/2}} U\left(\frac{|x|}{\sqrt{Dt}}\right) dx = 1$$

Substituting our ansatz $u^*(x, t) = \frac{1}{(Dt)^{n/2}} U\left(\frac{|x|}{\sqrt{Dt}}\right)$ in the homogeneous heat equation, we get

$$\begin{aligned} u_t^* &= \frac{1}{D^{n/2}} \left(-\frac{n}{2} t^{-n/2-1} U\left(\frac{|x|}{\sqrt{Dt}}\right) + \frac{1}{(Dt)^{n/2}} U'\left(\frac{|x|}{\sqrt{Dt}}\right) \frac{|x|}{\sqrt{D}} \left(-\frac{1}{2}\right) \frac{1}{t^{3/2}} \right) \\ &= -\frac{1}{2t(Dt)^{n/2}} (nU(\xi) + \xi U'(\xi)) \end{aligned}$$

as well as

$$\begin{aligned} u_{x_i} &= \frac{1}{(Dt)^{n/2}} \frac{1}{\sqrt{Dt}} \frac{2x_i}{|x|} \frac{1}{2} U'(\xi) \\ u_{x_i x_i} &= \frac{1}{(Dt)^{n/2}} \frac{1}{\sqrt{Dt}} \left(\frac{1}{|x|} - \frac{1}{2} \frac{2x_i^2}{|x|^3} \right) U'(\xi) + \frac{1}{(Dt)^{n/2}} \left(\frac{1}{\sqrt{Dt}} \right)^2 U''(\xi) \left(\frac{x_i}{|x|} \right)^2 \end{aligned}$$

Summing over i to express the Laplacian, we get

$$\begin{aligned} \sum_{i=1}^n u_{x_i x_i} &= \frac{1}{(Dt)^{n/2}} \frac{1}{\sqrt{Dt}} \left(\frac{n}{|x|} - \sum_{i=1}^n \frac{x_i^2}{|x|^3} \right) U'(\xi) + \sum_{i=1}^n \frac{1}{(Dt)^{n/2}} \frac{1}{Dt} U''(\xi) \frac{x_i^2}{|x|^2} \\ &= \frac{1}{(Dt)^{n/2+1}} \left(\frac{n-1}{\xi} U'(\xi) + U''(\xi) \right) \end{aligned}$$

Combining u_t and Δu into the heat equation, we get

$$0 = \frac{D}{(Dt)^{n/2+1}} \left(\frac{n-1}{\xi} U'(\xi) + U''(\xi) \right) + \frac{1}{2t} \frac{1}{(Dt)^{n/2}} (nU(\xi) + \xi U'(\xi)) \quad (16)$$

$$= \frac{n-1}{\xi} U'(\xi) + U''(\xi) + \frac{1}{2} (nU(\xi) + \xi U'(\xi)) = 0 \quad (17)$$

$$= (n-1)U'(\xi) + \xi U''(\xi) + \frac{n\xi}{2} U(\xi) + \frac{\xi^2}{2} U'(\xi) \quad (18)$$

An interesting aspect of (18) is that in this equation, in each pair of terms (first and second, and then third and last), when the order of the derivative in U is larger, the power of ξ is also larger.

Given this observation, it seems tantalizing to look for a matching expression of the form

$$(U'(\xi)\xi)' + (U(\xi)\xi^2)' = 0$$

The problem we unfortunately face is that in each of the pairs, one of the terms has a prefactor in n and the other hasn't. The term that is premultiplied by n is however always the lowest order term in ξ . In fact we see that the term without ξ contains a $(n-1)$ prefactor so that it seems tempting to multiply that term by ξ^{n-2} . From this we get

$$(n-1)\xi^{n-2}U'(\xi) + \xi^{n-1}U''(\xi) + \frac{n\xi^{n-1}}{2}U(\xi) + \frac{\xi^n}{2}U'(\xi) = 0$$

which can further be written as

$$\left(\xi^{n-1}U'(\xi)\right)' + \left(\frac{\xi^n}{2}U(\xi)\right)' = 0$$

Integrating, we get

$$\xi^{n-1}U'(\xi) + \frac{\xi^n}{2}U(\xi) = \text{constant}$$

Since this must be true for all ξ , if we assume $U'(0)$ and $U(0)$ to be finite, we necessarily have constant = 0 and hence $U' + \frac{1}{2}\xi U = 0$ or $U'/U = -\frac{1}{2}\xi$. Integrating this last expression, we get

$$\log U(\xi) = -\frac{1}{4}\xi^2 + C$$

which finally gives the expression of U : $U(\xi) = Ae^{-\frac{\xi^2}{4}}$.

Enforcing the conservation of mass fixes the remaining degree of freedom in the constant A ,

$$1 = \frac{1}{(Dt)^{n/2}} \int_{\mathbb{R}^n} U\left(\frac{|x|}{\sqrt{Dt}}\right) dx = \frac{A}{(Dt)^{n/2}} \int_{\mathbb{R}^n} e^{-\frac{1}{4}\frac{|x|^2}{Dt}} dx$$

To simplify the integral, we use the fact that the total mass of the multivariate Normal distribution is one, i.e.

$$\frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \int_{\mathbb{R}^n} e^{-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)} dx = 1$$

Letting $\Sigma = 2Dt\mathbf{I}$ where \mathbf{I} is the identity matrix, we get $|\Sigma| = (2Dt)^n$ and hence

$$1 = \frac{A}{(Dt)^{n/2}}(Dt)^{n/2}(4\pi)^{n/2} = 1$$

This last expression gives the value $A = (4\pi)^{n/2}$ for our normalizing constant. Our final expression for the fundamental solution can thus be summarized as follows

The function $\Phi(x, t)$ defined as

$$\Phi(x, t) = \frac{1}{(4\pi Dt)^{n/2}} \exp\left(-\frac{|x|^2}{4Dt}\right) \quad (19)$$

is called the [fundamental solution](#) of the diffusion/heat equation.

General remarks

First note that for $x \neq 0$

$$\lim_{t \rightarrow 0^+} \Phi(x, t) = \lim_{t \rightarrow 0^+} \frac{1}{(4\pi Dt)^{n/2}} \exp\left(-\frac{|x|^2}{4Dt}\right) = 0$$

while

$$\lim_{t \rightarrow 0^+} \Phi(0, t) = \lim_{t \rightarrow 0^+} \frac{1}{(4\pi Dt)^{n/2}} = +\infty$$

together, those facts indicate that if we interpret Φ as a probability density, when $t \rightarrow 0^+$, the fundamental solution tends to concentrate mass around the origin.

The limiting density distribution can be mathematically modeled by the so-called Dirac distribution (or measure) at the origin. The Dirac distribution is not a function in the usual sense as it satisfies

$$\begin{cases} \delta(0) = +\infty, & \delta(x) = 0 \quad \text{for } x \neq 0 \\ \int_{\mathbb{R}} \delta(x) dx = 1 \end{cases}$$

Providing a formal definition of the Dirac measure requires elements from the theory of distributions. In this lecture, we will restrict ourselves to heuristic considerations.

Let us focus our attention on the function

$$H(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases}$$

the characteristic function of the interval $[0, +\infty]$, known as the Heaviside (step) function. Observe that

$$\frac{H(x + \varepsilon) - H(x - \varepsilon)}{2\varepsilon} = \begin{cases} \frac{1}{2\varepsilon} & \text{if } -\varepsilon \leq x \leq \varepsilon \\ 0 & \text{otherwise} \end{cases} \quad (20)$$

if we denote this quotient as Q_ε , note that it satisfies the following properties. First

$$\int_{\mathbb{R}} Q_\varepsilon(x) dx = \frac{1}{2\varepsilon} 2\varepsilon = 1 \quad (21)$$

Moreover

$$\lim_{\varepsilon \rightarrow 0} Q_\varepsilon(x) = \begin{cases} 0 & \text{if } x \neq 0 \\ \infty & \text{if } x = 0 \end{cases} \quad (22)$$

Finally, for any smooth function $\varphi(x)$ (known as a test function) vanishing outside a bounded interval,

$$\int_{\mathbb{R}} Q_\varepsilon(x) \varphi(x) dx = \frac{1}{2\varepsilon} \int_{-\varepsilon}^{\varepsilon} \varphi(x) dx \xrightarrow{\varepsilon \rightarrow 0} \varphi(0) \quad (23)$$

Properties (21) and (22) above are identical to the properties of the Dirac distribution. Property (23) suggests that this object can be identified through its action on test functions.

We are now ready to provide a more rigorous definition the Dirac distribution

Definition 1. We call *Dirac measure* at 0, the generalized function denoted by δ that acts on a test function φ as

$$\delta[\varphi] = \varphi(0) \tag{24}$$

which is equivalently written as $\langle \delta, \varphi \rangle = \varphi(0)$ or even

$$\int_{\mathbb{R}} \delta(x)\varphi(x) dx = \varphi(0) \tag{25}$$

Note that we also have $Q' = \delta$. With this notion of Dirac distribution, we can thus say that our fundamental solution $\Phi(x)$ satisfies the initial conditions $\Phi(x, 0) = \delta(x)$

By translation invariance, the solution $\Phi(x - y, t)$ is also a solution of the diffusion equation that satisfies $\Phi(x - y, 0) = \delta(x - y)$

From the expression of Φ , we again see that initially the distribution Φ is zero outside the origin. As soon as $t > 0$, Φ becomes positive everywhere which amounts to saying that the unit mass diffuses instantaneously all over the space.

References

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