Chapter 5

Linear diffusion

5.1 The fundamental solution

The aim of this section is to derive the fundamental solution to the diffusion equation

$$\frac{\partial u}{\partial t} = d\frac{\partial^2 u}{\partial x^2}, \quad x \in \mathbb{R}, \;\; t \geq 0, \tag{5.1.1}$$

subject to far out boundary conditions

$$u(t, \pm\infty) = 0, \quad t \geq 0, \tag{5.1.2}$$

using *dimensional analysis*. This technique often reveals the basic structure of solutions to partial differential equations, by simply asking which (combination) of the variables actually determine the dependent variable we want to study.

Let us model the concentration of some species living on the real line, dispersing according to (5.1.1). Assume that at time $t = 0$, all individuals are in one particular location $x = 0$. Since the number of individuals remains constant in time, we know that for each $t > 0$,

$$\int_{-\infty}^{\infty} u(t, x)dx = 1. \tag{5.1.3}$$

(Exploiting the linearity of the diffusion equation, we have just taken the liberty of scaling u such that (5.1.3) holds.) A solution u is now completely determined by all other quantities involved, so we are looking for a function f such that

$$u = f(t, x, d). \tag{5.1.4}$$

We have already seen in Section 4.3 that (5.1.1) is invariant under the scaling $t^* = \varepsilon^2 t$, $x^* = \varepsilon x$. This suggests that we could write f as a function of $x/\sqrt{t}$. However, x^2/t is not dimensionless, and we therefore cannot expect solutions to be dependent on $x/\sqrt{t}$ *only*. Observe, however, from (5.1.1) that the diffusion constant d has dimension (length)^2/time. So the combination $x/\sqrt{dt}$ *is* dimensionless.

On the other hand, u has dimension 1/length, so we at least need f to be of the form $w\phi(x/\sqrt{dt})$ for some function w with dimension 1/length and a dimension-less function ϕ. The conservation equation (5.1.3) now yields

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} u(t, x)dx \\ &= \int_{-\infty}^{\infty} w\phi\left(\frac{x}{\sqrt{dt}}\right)dx \\ &= \int_{-\infty}^{\infty} w\sqrt{dt}\phi(\xi)d\xi, \end{aligned}$$

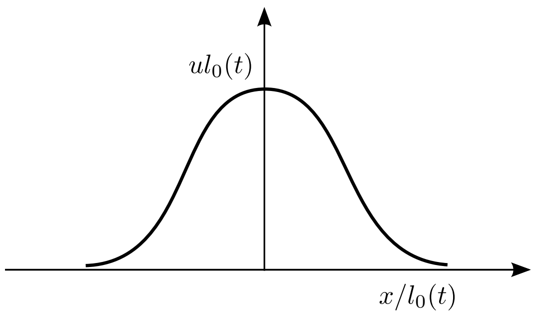

FIGURE 5.1. In the right time-dependent variables ($x/l_0(t)$ and $ul_0(t)$ the fundamental solution of the diffusion equation has a unique profile for all time.

where $\xi = x/\sqrt{dt}$. So $w = 1/\sqrt{dt}$ seems the obvious candidate to make all dimensions fit. In all, we look for a u of the form

$$u = \frac{1}{\sqrt{dt}}\phi\left(\frac{x}{\sqrt{dt}}\right).$$

This strategy of finding the structure of solutions by considering dimensions is applicable much more generally (Barenblatt, 1996).

Note that if we define the time-dependent length scale $l_0(t) := \sqrt{dt}$, then

$$u = \frac{1}{l_0(t)}\phi\left(\frac{x}{l_0(t)}\right),$$

so if we plot $ul_0(t)$ versus $x/l_0(t)$, we find *one* curve for all time. See Figure 5.1. This shows that this solution possesses the property of *self-similarity*: when scaling both the spatial variable and the (population) density in an appropriate time-dependent manner, nothing changes at all. In fact one can also find the form of the solution by, from the very beginning, searching for a solution such that

$$u(t,x) = \lambda^\alpha u(\lambda t, \lambda^\beta x) \quad \text{for all } \lambda > 0,$$

and constants α and β to be chosen suitably. The choice $\lambda = t^{-1}$ then reveals that we are looking for a function of one variable.

The great advantage of having to find $\phi(\xi)$ instead of $f(t,x,d)$ is that the (partial differential) diffusion equation (5.1.1) reduces to an *ordinary* differential equation in which, moreover, neither the independent nor the dependent variable carries a physical dimension.

EXERCISE 5.1.1. Show that, in the new variable ξ, (5.1.1) becomes

$$\frac{d^2\phi}{d\xi^2} + \frac{\xi}{2}\frac{d\phi}{d\xi} + \frac{\phi}{2} = 0. \tag{5.1.5}$$

Integrating once, we find that

$$\frac{d\phi}{d\xi} + \frac{\xi}{2}\phi = \text{constant}. \tag{5.1.6}$$

Since u is symmetric with respect to reflection in 0, ϕ should be symmetric around $\xi = 0$, and therefore $\frac{d\phi}{d\xi} = 0$ at $\xi = 0$. The constant on the right hand side is therefore zero. Using for instance integrating factors to solve (5.1.6), we conclude that

$$\phi(\xi) = Ae^{-\xi^2/4}, \tag{5.1.7}$$

for some constant A.

Using the well-known integral identity

$$\int_{\mathbb{R}} e^{-\xi^2} d\xi = \sqrt{\pi}.$$

we finally arrive at a solution of the diffusion equation, which we denote by Φ and which is explicitly given by the formula

$$\Phi = \frac{1}{2\sqrt{\pi dt}} e^{-\frac{x^2}{4dt}}.$$

We call Φ the *fundamental solution*. Note that $\Phi > 0$ for arbitrary x, no matter how small we choose $t > 0$. This is yet another manifestation of the infinite speed of propagation that is embodied in the diffusion equation. Also note that Φ is a Gauss distribution with mean zero and variance $2dt$. In particular, Φ is astronomically small for large $|x|$. So it is not so clear how we should interpret the positivity of Φ. We return to the question of the speed of propagation in Section 5.3 below. Finally note that the variance goes to zero for $t \downarrow 0$. So the distribution at $t = 0$ corresponds to a unit (recall (5.1.3)) mass concentrated at $x = 0$. In the mathematically precise sense of distributions, $u(t, .)$ converges to the Dirac delta for $t \downarrow 0$.

The reason Φ is called the *fundamental solution* is that by linearity of the diffusion equation we may apply *superposition*: given initial data $u(0, x) = u_0(x)$, the solution of the diffusion problem can be expressed as a convolution of the initial data and the fundamental solution:

$$u(t, x) = \int_{-\infty}^{\infty} \Phi(t, x - y) u_0(y) dy.$$

This section is greatly inspired by (Barenblatt, 1996, Section 2.1).

5.2 Separation of variables and spectral theory

If $\frac{du}{dt} = ru$ we know that u grows exponentially when $r > 0$, while it decays exponentially if $r < 0$. Now suppose that, additionally, u diffuses in a spatial domain. Is the conclusion still true? Does u develop any spatial pattern? What is the influence of boundary conditions? For simplicity we restrict our attention to a one-dimensional spatial domain. To begin with we provide the *diffusion equation*

$$\frac{\partial u}{\partial t} = d\frac{\partial^2 u}{\partial x^2} + ru \tag{5.2.1}$$

with so-called no-flux boundary conditions

$$\frac{\partial u}{\partial x}(t, 0) = 0 = \frac{\partial u}{\partial x}(t, L) \tag{5.2.2}$$

at the endpoints $x = 0$ and $x = L$ of the interval we consider.

EXERCISE 5.2.1. Explain why we can, without any loss of generality, either take $d = 1$ or $L = 1$. Also explain why, for $r > 0$, it is no loss of generality to take $r = 1$.

We choose to take $d = 1$, but to keep r as it is (so we scale the spatial variable but we do not scale time).

EXERCISE 5.2.2. Show that, in order for

$$u(t, x) = a(t)\phi(x)$$

to be a solution, we must necessarily have that, for some λ,

$$a(t) = \text{constant} \cdot e^{\lambda t},$$

and

$$\phi''(x) = (\lambda - r)\phi(x) \tag{5.2.3}$$
$$\phi'(0) = 0 = \phi'(L). \tag{5.2.4}$$

EXERCISE 5.2.3. Show that

(i) both $\phi(x) = \cos \mu x$ and $\phi(x) = \sin \mu x$ satisfy the differential equation $\phi'' = (\lambda - r)\phi$, provided $\lambda - r = -\mu^2$.
(ii) only $\phi(x) = \cos \mu x$ satisfies, in addition, the left boundary condition $\phi'(0) = 0$.
(iii) in order for $\phi(x) = \cos \mu x$ to also satisfy the right boundary condition $\phi'(L) = 0$, we should have
$$\mu = \frac{k\pi}{L} \quad \text{for some integer } k \geq 0.$$
(iv) finally, verify that (5.2.3)–(5.2.4) does *not* have a solution if $\lambda - r > 0$.

EXERCISE 5.2.4.

(i) Verify that, while making the preceding two exercises, you have deduced that the following statement is true: for $k = 0, 1, 2, \ldots$,
$$u(t,x) = e^{rt} e^{-\left(\frac{k\pi}{L}\right)^2 t} \cos\left(\frac{k\pi}{L} x\right) \tag{5.2.5}$$
is a solution of (5.2.1)—(5.2.2).
(ii) A very simple argument shows that of all these solutions the one with $k = 0$ has the fastest growth (or the least decay, when $r < 0$) for $t \to \infty$. Formulate this argument.
(iii) An even simpler argument shows that the solution with $k = 0$ is "flat", i.e., has no spatial structure. Provide also this argument.

The spatial solutions found in (5.2.5) can be used as building blocks for a representation of the general solution. By "general solution" we mean that we add to (5.2.1)—(5.2.2) an *initial condition*

$$u(0,x) = u_0(x), \tag{5.2.6}$$

where u_0 is a rather arbitrary function defined on $[0, L]$. Suppose that we can find coefficients $\{b_k\}_{k=0}^{\infty}$ such that

$$u_0(x) = \sum_{k=0}^{\infty} b_k \cos\left(\frac{k\pi}{L} x\right). \tag{5.2.7}$$

Then, by the superposition principle, which holds since (5.2.1)—(5.2.2) is a linear problem, and (5.2.5) we have

$$u(t,x) = e^{rt} \sum_{k=0}^{\infty} b_k e^{-\left(\frac{k\pi}{L}\right)^2 t} \cos\left(\frac{k\pi}{L} x\right). \tag{5.2.8}$$

The justification of (5.2.7) is the subject of Fourier analysis.

EXERCISE 5.2.5.

(i) In the above introduction of Section 5.2 we formulated three questions. Provide answers to the first two of these.
(ii) Alternatively to the no-flux boundary conditions (5.2.2), we can consider the situation in which the concentration is held zero at the boundary (imagine a big monster at the boundary that eats everything that gets there):
$$u(t,0) = 0 = u(t,L). \tag{5.2.9}$$

It follows that now

$$u(t,x) = e^{rt} \sum_{k=1}^{\infty} a_k e^{-\left(\frac{k\pi}{L}\right)^2 t} \sin\left(\frac{k\pi}{L}x\right). \tag{5.2.10}$$

Answer the first two questions in the introduction of this section for this situation. Hint: note that the term with $k = 0$ is now missing, as $\sin 0 = 0$.

(iii) Give a (partial) answer to the third question in the introduction.

Exercise 5.2.6. Consider a rectangular domain Ω with sides of length L_1 and L_2. Determine the eigenvalues and eigenvectors of the diffusion problem with no-flux boundary conditions. Conclude that the modes are naturally numbered by a *pair* of integers. If one orders the eigenvalues according to μ_{k_1,k_2}, one obtains an ordering of these pairs. Investigate the influence of the ratio L_1/L_2 on this ordering of pairs.

5.2.1 A digression on general theory

For general bounded open subsets Ω of $\mathbb{R}^n$, the eigenfunctions of the Laplace operator provided with zero Dirichlet boundary conditions form an orthonormal basis for $L^2(\Omega)$, i.e., every element f of $L^2(\Omega)$ can be written as

$$f = \sum_{i=1}^{\infty} \langle f, v_i \rangle v_i,$$

with $\Delta v_i = \lambda_i v_i$ for $i = 1, 2, \ldots$ The eigenvalues λ_i are real and negative and $\lambda_i \to -\infty$ as $i \to \infty$. The eigenvalue λ_1 is simple and the corresponding eigenfunction v_1 is positive (if we make the right choice; note that $-v_1$ is also an eigenfunction, so "is of one sign" is a slightly more accurate formulation). In fact, this positivity characterizes v_1: if $\lambda_i \neq \lambda_1$ then v_i cannot be chosen to be positive!

A cautionary note: often results are states for $-\Delta$ and then the eigenvalues are positive and converge to $+\infty$ for $i \to \infty$.

One can prove this result by first showing that a Green's function exists, and next using this function to convert the boundary value problem for the differential equation into an integral equation. Then general spectral theory of compact self-adjoint operators can be used. The positivity follows via the Krein-Rutman theorem, which is the infinite-dimensional version of Perron-Frobenius.

The idea of a *principal eigenvalue* with corresponding positive eigenfunction extends to operators of the form $Lu = \Delta u + ru$ where r is a function of x, rather than a scalar. To determine the sign of the principle eigenvalue (in order to decide about growth or decline) is a nontrivial task.

In the case of a one-dimensional spatial variable, this is part of the so-called Sturm-Liouville theory. The no-flux boundary condition is treated just as easily as the zero Dirichlet case (just compare the Exercises 5.2.4 and 5.2.5).

For higher dimensional Ω, one needs a bit of regularity of $\partial\Omega$ when dealing with no-flux boundary conditions. It is remarkably hard to find a precisely formulated result for the case of a no-flux boundary condition in the literature. After extensive searching we found Chapter 11, §A in Smoller (1983).

Finally, note that there also exist variational characterizations of the eigenvalues and eigenfunctions and these are particularly useful for dealing with the principal eigenvalue.

5.3 The asymptotic speed of propagation

This exercise is, in a way, a continuation of the preceding one. But now we consider a biological population living in a very large domain. In fact, the domain is so large that we use the plane $\mathbb{R}^2$ as an idealised mathematical description. So consider

$$\frac{\partial u}{\partial t} = d\Delta u + ru, \quad r > 0, \tag{5.3.1}$$

where $\Delta u = \frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2}$ and $x = (x_1, x_2) \in \mathbb{R}^2$. There are many situations in which one wants to know how fast the area occupied by the population expands. We shall derive the answer in two quite different ways. The first consists of analysing the fundamental solution

$$u(t,x) = \frac{1}{4\pi dt} e^{rt - \frac{|x|^2}{4dt}}, \quad \text{where } |x|^2 = x_1^2 + x_2^2. \tag{5.3.2}$$

describing the effect of a release at $t = 0$ at $x = 0$. The second relies on a search for travelling plane wave solutions, i.e., solutions of the form

$$u(t,x) = w(x \cdot \nu - ct), \tag{5.3.3}$$

where $w : \mathbb{R} \to \mathbb{R}$ defines the *profile*, the unit vector $\nu \in \mathbb{R}^2$ the *direction* and the real number c the *speed*.

EXERCISE 5.3.1. With u given by (5.3.2), for fixed x we have $\lim_{t\to\infty} u(t,x) = \infty$, while for fixed t we have $\lim_{|x|\to\infty} u(t,x) = 0$. To find out where, roughly, the transition from 0 to ∞ is located, we can consider $\lim_{t\to\infty} u(t,x)$ under various assumptions about how fast $|x(t)| \to \infty$ as $t \to \infty$.

(i) Show that this limit equals zero if $|x(t)|^2 > (4dr + \varepsilon)t^2$ for some $\varepsilon > 0$.
(ii) Show that, on the other hand, this limit equals ∞ if $|x(t)|^2 < (4dr - \varepsilon)t^2$ for some $\varepsilon > 0$.
(iii) Give arguments in favour of the assertion: "the population expands with speed $2\sqrt{dr}$".
(iv) Substitute (5.3.3) into (5.3.1) and derive an equation for w in which c figures as an additional (to d and r) parameter. Why did the ν drop out?
(v) Try for w an exponential function. Express the exponent in terms of c, r and d.
(vi) The biological interpretation requires w to be positive. This condition leads to a lower bound for the wave speed c. Which bound is this?
(vii) Comparing answers to (iii) and (vi), you find that the minimal speed of plane wave solutions coincides with the population expansion speed as derived from (5.3.2). Can you give an intuitive argument why this is to be expected? Hint: think in terms of fireworks that are ignited by fuses that we make as long or short as we want but that can also, via connections, be ignited by nearest neighbours.
(viii) Consider the plane wave solution with minimal speed. Check that at a fixed position the population grows like e^{2rt}, whereas a uniform (i.e., position independent) population grows as e^{rt}. Can you explain where the difference stems from?

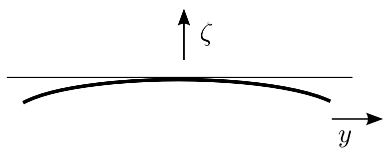

FIGURE 5.2.

We conclude this section with a more general look at the speed of propagation, without using the travelling wave Ansatz. Let us try to zoom in at the transition region by choosing a fixed direction ζ of unit length, and write $x = \alpha(t)\zeta + y$, with

$\zeta \cdot y = 0$, where α is a "local" one- dimensional coordinate corresponding to the ζ direction (Figure 5.2). With these assumptions, $|x|^2 = \alpha^2 + |y|^2$, and hence

$$u(t,x) = \frac{1}{4\pi dt} e^{rt\left(1-\frac{\alpha^2}{4rdt^2}\right)} e^{-\frac{|y|^2}{4dt}}.$$

For y in a bounded set, the last factor converges to 1 uniformly as $t \to \infty$. We would like to know at what speed $\alpha(t)$ has to progress such that the limit will be different from both zero and infinity. Call this limit ψ. Put $\frac{1}{4\pi dt} e^{rt\left(1-\frac{\alpha^2}{4rdt^2}\right)} = \psi$. Then solving for α^2, we find

$$\alpha^2 = 4drt^2 \left(1 - \frac{\log 4\pi dt}{rt} - \frac{\log \psi}{rt}\right),$$

and hence

$$\alpha = 2\sqrt{dr}t - \sqrt{\frac{d}{r}} \left(\log(4\pi dt) - \log(\psi)\right) + \mathcal{O}\left(\frac{\log^2(t)}{t}\right).$$

We write this as $\alpha = m(t) + \theta + \mathcal{O}\left(\frac{\log^2(t)}{t}\right)$, with $\theta = -\sqrt{\frac{d}{k}} \log(\psi)$. The new function $m(t)$ satisfies the differential equation

$$\dot{m}(t) = 2\sqrt{dr} - \sqrt{\frac{d}{r}}\frac{1}{t}.$$

Thus we see that the speed at which α needs to proceed converges algebraically to $2\sqrt{dr}$. Note that $\theta = -\sqrt{\frac{d}{r}} \log(\psi) \iff \psi = e^{-\theta\sqrt{\frac{r}{d}}}$.

Since ζ is arbitrary, we conclude that the fundamental solution u decomposes into plane waves travelling in all directions with speed $2\sqrt{dr}$, and that these waves describe the transition from inside the critically growing ball ($\psi \to \infty$, $\theta \to -\infty$), to outside ($\psi \to 0$, $\theta \to \infty$).

Travelling waves derive from the combination of a homogeneous medium and time translation invariance. The waves (in particular, their speeds) are independent of the direction ζ since the medium is isotropic.

On finite but large domains we still can use *self-similar solutions* (here travelling waves) to describe the *intermediate asymptotics* when the details of the initial condition do not matter anymore while boundary conditions do not yet influence the dynamics in a substantial way. For "self-similar", see Grindrod, box E (Grindrod, 1991), but also the book by Barenblatt devoted to self-similarity and intermediate asymptotics (Barenblatt, 1996). For each c the equation is invariant with respect to a group of transformations

$$T_\varepsilon^c = \begin{cases} x & \to & x + \varepsilon c, \\ t & \to & t + \varepsilon, \\ u & \to & u. \end{cases}$$

Hence, given a solution we can generate other (possibly, but not necessarily, different) solutions by applying T_ε^c. A similarity solution is one for which the group orbit $T_\varepsilon^c u$ consists of only one point.