Partial Differential Equations* (TATA27)

David Rule

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Contents

*These lecture notes are a based on the book *Partial Differential Equations* by W.A Strauss.
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1 Preliminaries

1.1 Notation

You will be familiar with notation for derivatives from previous courses, in particular from Calculus and Multivariable Calculus, but let us refresh our memories.

Given a real-valued function g of one real variable ($g\colon E \to \mathbf{R}$ where $E \subset \mathbf{R}$), we denote the derivative of g at a point t in its domain E as

$$g'(t) = \dot{g}(t) = \frac{dg}{dt}(t) := \lim_{h\to 0} \frac{g(t+h) - g(t)}{h}.$$

For a function f of more than one real variable, say $f\colon D \to \mathbf{R}$ where $D \subset \mathbf{R}^3$, we have three possible partial derivatives and a menagerie of notation:

$$f'_x(x,y,z) = f_x(x,y,z) = \partial_1 f(x,y,z) = \partial_x f(x,y,z) = \frac{\partial f}{\partial x}(x,y,z) := \lim_{h\to 0} \frac{f(x+h,y,z) - f(x,y,z)}{h};$$
$$f'_y(x,y,z) = f_y(x,y,z) = \partial_2 f(x,y,z) = \partial_y f(x,y,z) = \frac{\partial f}{\partial y}(x,y,z) := \lim_{h\to 0} \frac{f(x,y+h,z) - f(x,y,z)}{h};$$
$$f'_z(x,y,z) = f_z(x,y,z) = \partial_3 f(x,y,z) = \partial_z f(x,y,z) = \frac{\partial f}{\partial z}(x,y,z) := \lim_{h\to 0} \frac{f(x,y,z+h) - f(x,y,z)}{h}.$$

Different authors have different preferences and each notation seems best suited to different situations, so it's good to be aware of them all.

Higher order derivates are denoted analogously, for example f_{xx}, $\partial_x \partial_y f$, $\partial^2 f / \partial y^2$, f_{xxy}, etc.

The vector formed of all the partial derivates of f is called the *gradient* of f. This is written

$$\nabla f := (\partial_1 f, \partial_2 f, \partial_3 f)$$

For a function $F \colon D \to \mathbf{R}^3$, we can consider the divergence of F:

$$\operatorname{div} F = \nabla \cdot F := \partial_1 F_1 + \partial_2 F_2 + \partial_3 F_3,$$

where $F = (F_1, F_2, F_3)$. We can also consider the curl of F:

$$\operatorname{curl} F = \nabla \times F := (\partial_2 F_3 - \partial_3 F_2, \partial_3 F_1 - \partial_1 F_3, \partial_1 F_2 - \partial_2 F_1)$$

1.2 Differential equations

A *differential equation* is an equation that involves an unknown function u and derivatives of u. If u is a function of one variable, then the equation is called an *ordinary differential equation (ODE)*. If u is a function of more than one variable, then the equation is a *partial differential equation (PDE)*. For example, $u' = u$ is an ordinary diffential equation, but $u_x + 4u_y = 0$ is a partial differential equation.

A function u which satisfies a differential equation is called a *solution* to the equation. For example $u(x) = e^x$ is a solution to the equation $u' = u$.

The *order* of a differential equation is the order of the highest derivative that appears in the equation. Thus all second-order partial differential equations in two variables takes the form

$$F(x, y, u, \partial_x u, \partial_y u, \partial_{xx} u, \partial_{xy} u, \partial_{yy} u) = 0.$$

For example, if $F(x, y, w_0, w_1, w_2, w_{11}, w_{12}, w_{22}) = w_{11} + w_{22}$, then the differential equation is $\partial_{xx} u + \partial_{yy} u = 0$.

We will find the notion of differential operator convenient to use. An *operator* is a function which maps functions to functions. A *differential operator* is an operator which takes derivatives of the function it acts on. For example, for a fixed $n \in \mathbf{N}$, ∇ is a differential operator which maps $f \colon \mathbf{R}^n \to \mathbf{R}$ to the function $\nabla f \colon \mathbf{R}^n \to \mathbf{R}^n$ given by the formula $\nabla f(\mathbf{x}) = (\partial_1 f(\mathbf{x}), \partial_2 f(\mathbf{x}), \ldots, \partial_n f(\mathbf{x}))$. It is often useful to use the notation introduced above to denote differential operators, for example the operator $u \mapsto u_t - u_{xx} = (\partial_t - \partial_x^2) u$ can be denoted simply as $(\partial_t - \partial_x^2)$.

An operator $\mathcal{L}$ is called *linear* if $\mathcal{L}(\alpha u + \beta v) = \alpha \mathcal{L}(u) + \beta \mathcal{L}(v)$ for all $\alpha, \beta \in \mathbf{R}$ and all functions u and v. It is easy to check the following operators are linear operators.

1. The gradient operator $\nabla = (\partial_1, \partial_2, \ldots, \partial_n)$ acting on functions $u \colon \mathbf{R}^n \to \mathbf{R}$.
2. Divergence div acting on functions $u \colon \mathbf{R}^n \to \mathbf{R}^n$ as $\operatorname{div} u = \sum_{j=1}^n \partial_j u_j$ where $u_j \colon \mathbf{R}^n \to \mathbf{R}$ are the component functions of u so $u = (u_1, u_2, \ldots, u_n)$.
3. curl acting on functions $u = (u_1, u_2, u_3) \colon \mathbf{R}^3 \to \mathbf{R}^3$ by the formula
$$\operatorname{curl}(u) = (\partial_2 u_3 - \partial_3 u_2, \partial_3 u_1 - \partial_1 u_3, \partial_1 u_2 - \partial_2 u_1).$$
4. The Laplacian $\Delta := \nabla \cdot \nabla = \sum_{j=1}^n \partial_j^2$ acting on $f \colon \mathbf{R}^n \to \mathbf{R}$.

An example of an operator which is not linear is $u \mapsto u_y + u_{xxy} + u u_x$. (Why?)

The *order* of an operator is the order of the differential equation $\mathcal{L}(u) = 0$ as an equation in u. A differential equation is said to be a *linear homogeneous* equation, if it is of the form $\mathcal{L}(u) = 0$, where $\mathcal{L}$ is a linear differential operator. It is said to be a *linear inhomogeneous* equation if it is of the form $\mathcal{L}(u) = f$ for some function f, where again $\mathcal{L}$ is a linear differential operator.

2 First-order linear equations and the method of characteristics

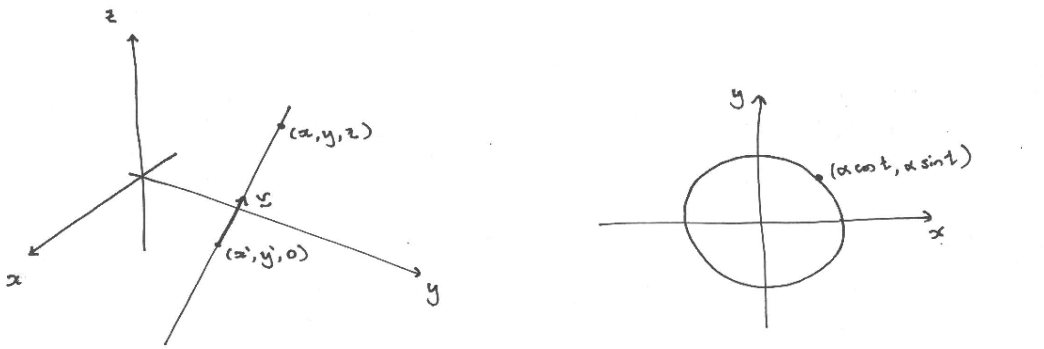
We shall begin by attempting to solve a fairly simple equation: Find all functions $u\colon \mathbf{R}^3 \to \mathbf{R}$ such that

$$au_x + bu_y + cu_z = 0 \quad \text{in } \mathbf{R}^3, \tag{2.1}$$

where a, b and c are three given constants not all zero. Although the equation itself is simple, to solve it we will use a method which is quite powerful. Observe that the equation can be rewritten as

$$\mathbf{v} \cdot \nabla u = 0$$

where $\mathbf{v} = (a, b, c)$. Thus the equation says that the directional derivate in the direction $\mathbf{v}/|\mathbf{v}|$ is zero. Thus any solution u will be constant along lines parallel to $\mathbf{v}$.



(a) An example of a line along which a solution u to (2.1) is constant.

(b) A characteristic curve along which a solution u to (2.2) is constant

Figure 1: Characteristic curves

Since we are assuming that at least one of a, b and c is non-zero, suppose for definitness that $c \neq 0$. Then the vector $\mathbf{v}$ has a component pointing out of the xy-plane and each point $(x, y, z) \in \mathbf{R}^3$ lies on a unique line parallel to $\mathbf{v}$ which passes through the xy-plane at a point $(x', y', 0)$ (see Figure 1(a)). Since we worked out that the solution u is constant along lines parallel to $\mathbf{v}$, we know $u(x, y, z) = u(x', y', 0)$. Moreover, the difference between (x, y, z) and $(x', y', 0)$ is some multiple $\alpha \in \mathbf{R}$ of $\mathbf{v}$. That is,

$$(x, y, z) - (x', y', 0) = \alpha(a, b, c).$$

Since $c \neq 0$, we have that $\alpha = z/c$, so $x' = x - za/c$ and $y' = y - zb/c$. Thus,

$$u(x, y, z) = u(x - za/c, y - zb/c, 0).$$

Finally, we observe that we are free to choose the value of the solution arbitrarily on the xy-plane, so the general solution to (2.1) is of the form

$$u(x, y, z) = f(x - za/c, y - zb/c).$$

Such a u will solve equation (2.1) provided both first-order partial derivates of $f\colon \mathbf{R}^2 \to \mathbf{R}$ exist.

The cases when $a \neq 0$ and $b \neq 0$ can be handled similarly.

2.1 The method of characteristics

Now we have solved (2.1) we can see that the key was to identify lines along which the solution was constant. Let us take this idea but apply it in a more abstract setting to solve a similar, but more complicated equation, this time in two variables. Consider the equation

$$xu_y(x, y) - yu_x(x, y) = 0 \quad \text{for } (x, y) \in \mathbf{R}^2 \setminus \{(0, 0)\}. \tag{2.2}$$

This is again a first-order linear equation, but this time with variable coefficients. We will look for lines in $\mathbf{R}^2 \setminus \{(0,0)\}$ along which the solution u is constant. Suppose these lines are parametrised by a variable t and the x-coordinate is given by the function $t \mapsto X(t)$ and the y-coordinate by $t \mapsto Y(t)$. Thus we know that

$$t \mapsto u(X(t), Y(t)) =: z(t) \text{ is a constant function}$$

Consequently, using the chain rule, we have that

$$0 = z'(t) = \frac{d}{dt} u(X(t), Y(t)) = X'(t) u_x(X(t), Y(t)) + Y'(t) u_y(X(t), Y(t)). \tag{2.3}$$

Comparing this with equation (2.2) we see that it is a good idea to choose

$$\begin{aligned} X'(t) &= -Y(t), \quad \text{and} \\ Y'(t) &= X(t), \end{aligned}$$

which have solutions $X(t) = \alpha \cos(t)$ and $Y(t) = \alpha \sin(t)$ for any $\alpha \in \mathbf{R}$ (see Figure 1(b)). Thus any solution to (2.2) is constant on circles centred at the origin and an arbitrary solution can be written in the form

$$u(x, y) = f(x^2 + y^2).$$

Such a function will solve (2.2) provided $f\colon (0, \infty) \to \mathbf{R}$ is differentiable. The curves

$$\{(x, y) | x = X(t),\ y = Y(t) \text{ for some } t \in \mathbf{R}\}$$

are called the *characteristic curves* (or more simply, the *characteristics*) of (2.2).

The method we employed here was to search for curves (called characteristic curves) on which the solution to our PDE behaved in a simple manner. In the previous two examples, the solution was constant on the characteristic curves, but, in principle, the solution only needs to behave in an understandable way along the characteristic curves—for example, it would suffice if $t \mapsto u(X(t), Y(t))$ satisfied an ODE we could easily solve. Let us look at another which demonstrates this more complicated situation.

Consider the equation

$$u_x(x, y) + \cos(x) u_y(x, y) = 1 \quad \text{for } (x, y) \in \mathbf{R}^2 \tag{2.4}$$

and suppose that we are given the value of u along the y-axis, say

$$u(0, y) = f(y) \tag{2.5}$$

for some differentable function $f\colon \mathbf{R} \to \mathbf{R}$ and all $y \in \mathbf{R}$. Once again we look for particular curves $t \mapsto (X(t), Y(t))$ but instead of requiring $z(t) := u(X(t), Y(t))$ is constant along these curves, we allow (2.4) to determine how z behaves. Using the chain rule,

$$z'(t) = \frac{d}{dt} u(X(t), Y(t)) = X'(t) u_x(X(t), Y(t)) + Y'(t) u_y(X(t), Y(t)).$$

Comparing this with the coefficients in front of the first order terms in (2.4), we take

$$X'(t) = 1, \quad \text{and} \tag{2.6}$$
$$Y'(t) = \cos(X(t)), \tag{2.7}$$

which means z satisfies the ODE

$$z'(t) = u_x(X(t), Y(t)) + \cos(X(t)) u_y(X(t), Y(t)) = 1. \tag{2.8}$$

The ODE (2.8) is a replacement for (2.3) in the previous example: z is not longer a constant function, where it satisfied $z'(t) = 0$, but instead satisfies a slightly more complicated ODE, $z'(t) = 1$, which we must also solve.

First we find the characteristic curves. We can solve (2.6) to obtain $X(t) = t + c_1$ for a constant c_1 and substituting this in (2.7), we have $Y'(t) = \cos(t+c_1)$, which implies $Y(t) = \sin(t+c_1)+c_2$. We now want to relate the solution $u(x, y)$ at an arbitrary point (x, y) with the solution at a point along the y-axis, where we know the solution is equal to f by (2.5). So we look for a characteristic curve which goes through the point (x, y) when $t = 0$. This is easy to find: we take $c_1 = x$ and $c_2 = y - \sin(x)$, so

$$\begin{aligned} X(t) &= t + x, \quad \text{and} \\ Y(t) &= \sin(t + x) + y - \sin(x). \end{aligned}$$

The curve $t \mapsto (X(t), Y(t)$ will intersect the y-axis when $0 = X(t) = t + x$, which occurs when $t = -x$. To relate $u(x, y)$ with $u(0, Y(-x))$ we calculate $\int_{-x}^{0} z'(t)dt$. By the Fundamental Theorem of Calculus,

$$\int_{-x}^{0} z'(t)dt = z(0) - z(-x) = u(X(0), Y(0)) - u(X(-x), Y(-x)) = u(x, y) - u(0, y - \sin(x)),$$

but, using (2.8), this is also

$$\int_{-x}^{0} z'(t)dt = \int_{-x}^{0} 1dt = x,$$

so we obtain $x = u(x, y) - u(0, y - \sin(x)) = u(x, y) - f(y - \sin(x))$, where we also used (2.5), and thus

$$u(x, y) = x + f(y - \sin(x)).$$

We can check directly that this is indeed a solution to (2.4) and satisfies (2.5).

The method of characteristics can be summarised as a method where we first look for particular curves $t \mapsto (X(t), Y(t))$ along which the solution to our PDE obeys a simple ODE — an ODE in the unknown $z(t) = u(X(t), Y(t))$ — and then solve this ODE. In the previous example, the characteristic curves were determined by (2.6)-(2.7). Hopefully there are sufficiently many curves so that there is always one connecting an arbitrary point (x, y) to a point where we have information about the solution (the y-axis in the previous example). We can then compare the solution at these two points by solving the ODE for z (this was the ODE (2.8) in our example).

3 The physical origins of some PDEs

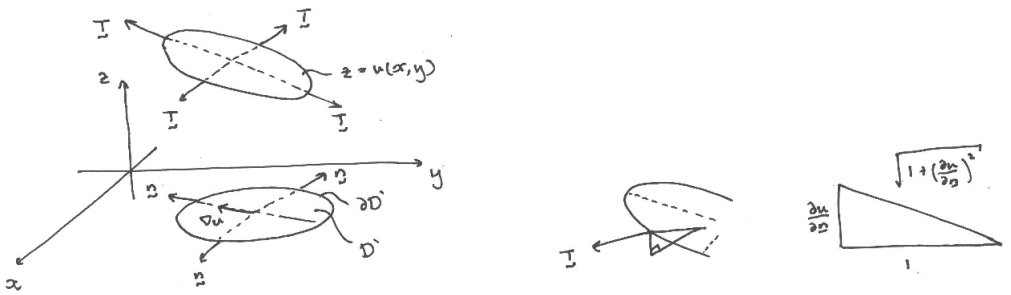
In this section we will give some physical motivation for the main equations we will study. We will not worry about being too careful in our derivation of the equations, but simply want to provide some physical context for why the equations are of interest. Our careful mathematical analysis will now be postponed until the next section, where we will take the equations as the starting point.

3.1 Vibrations and the wave equation

Let us consider a vibrating drumhead. Suppose that an elastic membrane is streached over a frame ∂D that lies in the xy-plane. For each point $\mathbf{x}$ inside the frame (a region D, so $\mathbf{x} \in D$) and time t we denote the displacement of the membrane by $u(\mathbf{x}, t)$. We wish to derive a simple equation that the function u satisfies in D which describes how the membrane behaves when subject to small displacements.

Assume the membrane has a mass density of ρ and is under constant tension (force per unit arclength) of magnitude T. Newton's second law says that the mass times the acceleration of a small part of the membrane D' is equal to the (vector) sum of the forces acting on that part. We will assume the membrane only moves in the vertical direction, so we are interested in the sum of the vectical components of the forces acting on a part of the membrane. The force of tension acts parallel to the surface of the membrane, so its vertical component at each point $\mathbf{x} \in \partial D'$ is proportional to

$$\frac{(\partial u/\partial \mathbf{n})}{\sqrt{1 + (\partial u/\partial \mathbf{n})^2}} \approx \frac{\partial u}{\partial \mathbf{n}} \quad \text{if } (\partial u/\partial \mathbf{n}) \text{ is small,}$$



(a) The tension $\mathbf{T}$ acting on the edge of a piece of the membrane acts in a direction parallel with both the tangent plane of the surface $z = u(x, y)$ and the plane containing the normal vector $\mathbf{n}$ to ∂D and the z-axis. We assume $|\mathbf{T}| = T$ is constant.

(b) To compute the vertical component of the tension at a point on the edge, consider the slope of $z = u(x, y)$ in the normal direction $\mathbf{n}$. This is equal to $\frac{T(\partial u/\partial \mathbf{n})}{\sqrt{1+(\partial u/\partial \mathbf{n})^2}}$ which is approximately $T\partial u/\partial \mathbf{n}$ when $\partial u/\partial \mathbf{n}$ is small.

Figure 2: Tension acting on a small piece of an elastic membrane

where $\mathbf{n}$ is the outward unit normal to $\partial D'$ and $\partial u/\partial \mathbf{n} = \mathbf{n} \cdot \nabla u$ is the normal derivative of u. The constant of proportionality is the tension T, so the total vertical force is the "sum" of this around the boundary $\partial D'$:

$$\int_{\partial D'} T \frac{\partial u}{\partial \mathbf{n}}(\mathbf{x}, t) d\sigma(\mathbf{x}).$$

(See Figure 2.) Newton's second law says this is equal to the mass times the acceleration of D'. Thus

$$\int_{\partial D'} T \frac{\partial u}{\partial \mathbf{n}}(\mathbf{x}, t) d\sigma(\mathbf{x}) = \iint_{D'} \rho u_{tt}(\mathbf{x}, t) d\mathbf{x}.$$

The divergence theorem says

$$\int_{\partial D'} T \frac{\partial u}{\partial \mathbf{n}}(\mathbf{x}, t) d\sigma(\mathbf{x}) = \iint_{D'} \operatorname{div}(T \nabla u(\mathbf{x}, t)) d\mathbf{x},$$

and so,

$$\iint_{D'} \operatorname{div}(T \nabla u(\mathbf{x}, t)) d\mathbf{x} = \iint_{D'} \rho u_{tt}(\mathbf{x}, t) d\mathbf{x}.$$

Since D' was arbitrary, we find that u satisfies

$$u_{tt}(\mathbf{x}, t) = c^2 \Delta u(\mathbf{x}, t) \quad \text{for all } \mathbf{x} \in D \text{ and } t \in R, \text{ where } c = \sqrt{\frac{T}{\rho}}. \tag{3.1}$$

The equation in (3.1) is called the *wave equation*

3.2 Diffusion and the heat equation

Let us consider two fluids which together fill a container. We are interested in how these two fluids will mix. Fick's law of diffusion states that

the flow of a fluid is proportional to the gradient of its concentration.

Let $u(\mathbf{x}, t)$ be the concentration of one fluid at a point $\mathbf{x}$ and time t. For an arbitrary region D' the mass of the fluid in D' is

$$m(t) = \iiint_{D'} u(\mathbf{x}, t) d\mathbf{x}, \quad \text{so} \quad \frac{dm}{dt}(t) = \iiint_{D'} u_t(\mathbf{x}, t) d\mathbf{x}.$$

The rate of change of mass of fluid in the region D' is also equal to the net flow of mass into the region D'. By Fick's law this is given by

$$\frac{dm}{dt}(t) = \iint_{\partial D'} k\mathbf{n} \cdot \nabla u(\mathbf{x}, t) d\sigma(\mathbf{x}).$$

Therefore using the divergence theorem, we obtain

$$\iiint_{D'} \operatorname{div}(k\nabla u)(\mathbf{x}, t) d\mathbf{x} = \iint_{\partial D'} k\mathbf{n} \cdot \nabla u(\mathbf{x}, t) d\sigma(\mathbf{x}) = \frac{dm}{dt}(t) = \iiint_{D'} u_t(\mathbf{x}, t) d\mathbf{x}.$$

Once again, since D' was abitrary, the integrands must also be equal:

$$u_t(\mathbf{x}, t) = k\Delta u(\mathbf{x}, t) \quad \text{for all } \mathbf{x} \text{ and } t. \tag{3.2}$$

Equation (3.2) is called the *diffusion* or *heat equation*.

3.3 Harmonic functions

When we consider solutions to both the heat and the wave equation ((3.2) and (3.1)) which are independent of time, we find that they are both solutions to *Laplace's equation*:

$$\Delta u(\mathbf{x}) = \sum_{j=1}^{n} \partial_j^2 u(\mathbf{x}) = 0 \tag{3.3}$$

Functions u which are solutions of (3.3) are called *harmonic* functions. When $n = 1$, the only such functions are linear functions $u(x) = kx + c$, but for $n > 1$ things become more interesting.

4 Boundary value problems and well-posedness

We have derived several different PDEs which model various physical situations, but we have also seen that there can be many different solutions to any one given PDE. If a PDE is to be a genuinely useful model, we would expect it to give exactly one possibility for a physical property (which the solution to the PDE represents). Thus, we must add some further conditions to the model that will pick out the solution which is physically relevant to a given situation. The precise conditions we have to add vary slightly depending on the model, but are usually motivated by physical considerations.

4.1 Function spaces

The function space where we look for a solution is a subtle issue, but important. For example, in quantum mechanics a solution $u\colon \mathbf{R}^3 \times \mathbf{R} \to \mathbf{C}$ to a PDE can be connected to the probability density of a particle. The probability that a particle lies in a region $D \subset \mathbf{R}^3$ at time t is given by

$$\int_D |u(\mathbf{x}, t)|^2 d\mathbf{x}.$$

Since it is a probability, we would expect $\int_{\mathbf{R}^3} |u(\mathbf{x}, t)|^2 d\mathbf{x} = 1$, and so any physically reasonable solution u is such that $\int_{\mathbf{R}^3} |u(\mathbf{x}, t)|^2 d\mathbf{x} = 1$ for all t.

4.2 Initial conditions

An *initial condition* specifies the solution at a particular instant of time. We typically use the variables $\mathbf{x} = (x, y, z)$ to denote spatial coordinates and t to denote a time coordinate. So an initial condition can take the form $u(\mathbf{x}, t_0) = f(\mathbf{x})$ for all $\mathbf{x} \in \mathbf{R}^n$ (and a given f). We would then search for a solution u which satisfies a given PDE for $t > t_0$. If we consider heat flow (or diffusion of a chemical), specifying the temperature (or concentration) at a specific time $t = t_0$, that is prescribing the solution $u(\cdot, t_0)$ at time t_0, ought to be sufficient to pin down a unique solution $u(\cdot, t)$ for $t > t_0$. Thus, the problem we

expect to be able to solve is, given a function $f\colon \mathbf{R}^3 \to \mathbf{R}$, to find a unique function $u\colon \mathbf{R}\times[t_0,\infty) \to \mathbf{R}$ such that

$$\begin{cases} \partial_t u(\mathbf{x},t) - k\Delta u(\mathbf{x},t) = 0 & \text{for } (\mathbf{x},t) \in \mathbf{R}^3 \times (t_0,\infty), \text{ and} \\ u(\mathbf{x},t_0) = f(\mathbf{x}) & \text{for } \mathbf{x} \in \mathbf{R}^3. \end{cases}$$

Observe that here the function space we assume u to lie in is also important. For example, if we do not require that u is continuous at $t = t_0$, the initial condition will not really limit the number of solutions we have. It can be useful to reformulate the initial condition to take the need for such continuity into account directly. For example,

$$\lim_{t\to t_0} u(\mathbf{x},t) = f(\mathbf{x}) \quad \text{for all } \mathbf{x} \in \mathbf{R}^3.$$

Sometimes it is reasonable to give two initial conditions, as is the case with the wave equation. Given $f\colon \mathbf{R}^3 \to \mathbf{R}$ and $g\colon \mathbf{R}^3 \to \mathbf{R}$, we expect to find a unique $u\colon \mathbf{R}^3 \times [t_0,\infty) \to \mathbf{R}$ such that

$$\begin{cases} \partial_t^2 u(\mathbf{x},t) - c^2\Delta u(\mathbf{x},t) = 0 & \text{for } (\mathbf{x},t) \in \mathbf{R}^3 \times (t_0,\infty), \text{ and} \\ u(\mathbf{x},t_0) = f(\mathbf{x}) \text{ and } \partial_t u(\mathbf{x},t_0) = g(\mathbf{x}) & \text{for } \mathbf{x} \in \mathbf{R}^3. \end{cases}$$

Here the initial conditions specify the position and velocity of u at time t_0.

4.3 Boundary conditions

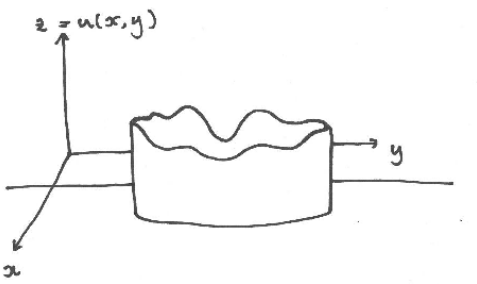


Figure 3: A cup with an uneven rim sitting on a table.

A *boundary condition* specifies the value of a solution on the boundary of (what physically is) a spatial domain. For example, take a cup which has an uneven rim, place it on a table and then stretch a rubber sheet over its rim (see Figure 3). One can show that the height of the rubber should roughly be given by a harmonic function (with respect to two variables — those of horizontal position over the table) and the height at the boundary would, of course, be the height of the rim. Thus, if D is (the interior of) the region of the table over which the cup sits, we would expect to be able to find a unique $u\colon \mathbf{R}^2 \to \mathbf{R}$ such that

$$\begin{cases} \Delta u(x,y) = 0 & \text{for all } (x,y) \in D, \text{ and} \\ u(x,y) = f(x,y) & \text{for } (x,y) \in \partial D. \end{cases}$$

Here ∂D denotes the boundary of D, that is, points above which the cup's rim sits, and $f(x,y)$ is the height of the cup's rim above the table at $(x,y) \in \partial D$.

4.4 Well-posedness

Once we believe we have formulated a physically sensible model, we then want to prove rigorously the following properties.

1. Existence: There exists at least one solution that satisfies the PDE together with the initial/boundary conditions and lies in our chosen function space.

2. Uniqueness: There exists at most one solution that satisfies the PDE together with the initial/boundary conditions and lies in our chosen function space.

3. Stability: The solution depends continuously on the data (that is, the initial/boundary conditions).

We impose the third condition as in practice we cannot measure our data exactly, so it is useful to know that any small error in measurement will only lead to a small change in the solution.

5 Laplace's and Poisson's equation

We said earlier that a solution to Laplace's equation (3.3) is called harmonic. We will also be interested in an inhomogeneous version of Laplace's equation. Namely, *Poisson's equation*:

$$\Delta u(\mathbf{x}) = \sum_{j=1}^{n} \partial_j^2 u(\mathbf{x}) = f(\mathbf{x}) \tag{5.1}$$

for a given function f.

5.1 A maximum principle

Maximum principles are very powerful analytic tool for studying harmonic functions. Recall that a set $D \subset \mathbf{R}^n$ is called *open* if for every point $\mathbf{x} \in D$, there exists an $\varepsilon > 0$ such that the set $\{\mathbf{y} \,|\, |\mathbf{x}-\mathbf{y}| < \varepsilon\}$ is a subset of D. A set $D \subset \mathbf{R}^n$ is called *bounded* if there exists a constant $C > 0$ such that $|\mathbf{x}| < C$ for all $\mathbf{x} \in D$.

Theorem 5.1 (Weak Maximum Principle)**.** *Let $\Omega \subset \mathbf{R}^n$ be a connected bounded open set. Let $u\colon \overline{\Omega} \to \mathbf{R}$ be a continuous function which is harmonic in Ω. Then the maximum and minimum values of u are attained on $\partial\Omega$.*

From a physical point of view, the Maximum Principle is fairly obvious. For example, a harmonic function is a stationary solution to the heat equation and one would not expect the hotest part of a body which has reached an equilibrium to be in the middle of the body.

It can also be motivated mathematically as follows. For example, if $n = 2$ and we have a maximum point $(x, y) \in \Omega$, then—as can been seen by looking at the second derivative test from Calculus—it is often the case that $u_{xx}(x, y) < 0$ and $u_{yy}(x, y) < 0$. This contradicts the fact that u is harmonic, which says $u_{xx}(x, y) + u_{yy}(x, y) = 0$. However, 'often' is not 'always', so we must work harder in order to actually prove the theorem.

Proof of Theorem 5.1. For $\varepsilon > 0$ set $v(\mathbf{x}) = u(\mathbf{x}) + \varepsilon|\mathbf{x}|^2$. As the sum of two continuous functions, v is continuous on $\overline{\Omega}$ and so must attain a maximum somewhere in the compact set $\overline{\Omega} = \Omega \cup \partial\Omega$. We will now rule out the possibility that v attains its maximum in Ω. Suppose to the contrary that v attains this maximum $\mathbf{x} \in \Omega$. Then, by the second derivative test, $\Delta v(\mathbf{x}) = \sum_{j=1}^{n} \partial_j^2 v(\mathbf{x}) \leq 0$. But on the other hand, we can compute

$$\Delta v = \Delta u + 2\varepsilon n = 2\varepsilon n > 0,$$

which contradicts $\Delta v(\mathbf{x}) \leq 0$, so v cannot attain its maximum in Ω. Therefore v must attain its maximum at a point $\mathbf{y} \in \partial\Omega$. Thus, for any $\mathbf{x} \in \overline{\Omega}$,

$$u(\mathbf{x}) \leq v(\mathbf{x}) \leq v(\mathbf{y}) = u(\mathbf{y}) + \varepsilon|\mathbf{y}|^2 \leq u(\mathbf{y}) + \varepsilon C^2 \leq \max_{\partial\Omega} u + \varepsilon C^2,$$

where C is the constant obtained from the fact D is bounded. Since the above inequality holds for any $\varepsilon > 0$, we have $u(\mathbf{x}) \leq \max_{\partial\Omega} u$ for any $\mathbf{x} \in \overline{\Omega}$, so

$$\max_{\overline{\Omega}} u \leq \max_{\partial\Omega} u$$

Because $\partial\Omega \subseteq \overline{\Omega}$ we have that $\max_{\partial\Omega} u \leq \max_{\overline{\Omega}} u$ and combining these two inequalities we get that $\max_{\overline{\Omega}} u = \max_{\partial\Omega} u$ and the maximum of u is attained on $\partial\Omega$. (Observe that we have not ruled out the possibility that the maximum of u is also attained in Ω — that we only managed to do for v — so it may still be possible that the maximum of u is attained both in Ω and on $\partial\Omega$.)

That the minimum is attained on the boundary $\partial\Omega$ can be proved similarly. □

5.2 Uniqueness for the Dirichlet problem

We can use the Weak Maximum Principle to prove that a solution to the Dirichlet problem for the Poisson equation is unique.

Suppose we had two functions u_1 and u_2 which where continuous on $\overline{\Omega}$, for an connected bounded open set $\Omega \subset \mathbf{R}^n$ and such that (for $i = 1, 2$)

$$\begin{cases} \Delta u_i = f & \text{in } \Omega, \text{ and} \\ u_i = g & \text{on } \partial\Omega, \end{cases} \tag{5.2}$$

where $g\colon \partial\Omega \to \mathbf{R}$ and $f\colon \Omega \to \mathbf{R}$.

The difference $w := u_2 - u_1$ is continuous on $\overline{\Omega}$ and satisfies

$$\begin{cases} \Delta w = 0 & \text{in } \Omega, \text{ and} \\ w = 0 & \text{on } \partial\Omega, \end{cases}$$

We can apply Theorem 5.1 to conclude that both the maximum and the minimum of w are obtained on the boundary of $\partial\Omega$, but by the boundary condition we know

$$0 = \min_{\partial\Omega} w \leq w(\mathbf{x}) \leq \max_{\partial\Omega} w = 0$$

for any $\mathbf{x} \in \overline{\Omega}$. Thus $w \equiv 0$ and so $u_1 = u_2$, that is to say, there is at most one continuous solution $u\colon \overline{\Omega} \to \mathbf{R}$ of the boundary value problem

$$\begin{cases} \Delta u = f & \text{in } \Omega, \text{ and} \\ u = g & \text{on } \partial\Omega, \end{cases}$$

for $g\colon \partial\Omega \to \mathbf{R}$ and $f\colon \Omega \to \mathbf{R}$. Observe that we did not need to make any regularity assumptions about f or g, although obviously g may inherit continuity from the fact we assumed u was continuous.

5.3 Laplace's equation in two dimensions

To further investigate the properties of harmonic functions it is instructive to first restrict our attention to $n = 2$, so $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$.

5.3.1 The Laplacian in polar coordinates

We wish to use polar coordinates to rewrite the Laplace operator (Laplacian) in terms of $\partial/\partial r$ and $\partial/\partial\theta$. The transformation from polar to Cartesian coordinates is given by

$$x = r\cos\theta \quad \text{and} \quad y = r\sin\theta$$

and the inverse is[1]

$$r = \sqrt{x^2 + y^2} \quad \text{and} \quad \theta = \arctan(y/x)$$

Recall that the chain rule says

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta} \quad \text{and} \quad \frac{\partial}{\partial y} = \frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial y}\frac{\partial}{\partial\theta}$$

[1]The formula $\theta = \arctan(y/x)$ is not quite the inverse, as θ may lie outside the range $(-\pi/2, \pi/2)$.

so we obtain

$$\frac{\partial}{\partial x} = \cos\theta \frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial \theta} \quad \text{and} \quad \frac{\partial}{\partial y} = \sin\theta \frac{\partial}{\partial r} + \frac{\cos\theta}{r}\frac{\partial}{\partial \theta}$$

Squaring these operators, we obtain

$$\begin{aligned}\frac{\partial^2}{\partial x^2} &= \left(\cos\theta \frac{\partial}{\partial r} + \frac{\sin\theta}{r}\frac{\partial}{\partial \theta}\right)^2 \\ &= \cos^2\theta \frac{\partial^2}{\partial r^2} - 2\left(\frac{\sin\theta\cos\theta}{r}\right)\frac{\partial^2}{\partial r \partial\theta} + \frac{\sin^2\theta}{r^2}\frac{\partial^2}{\partial\theta^2} + 2\left(\frac{\sin\theta\cos\theta}{r^2}\right)\frac{\partial}{\partial\theta} + \frac{\sin^2\theta}{r}\frac{\partial}{\partial r}\end{aligned}$$

and

$$\begin{aligned}\frac{\partial^2}{\partial y^2} &= \left(\sin\theta \frac{\partial}{\partial r} + \frac{\cos\theta}{r}\frac{\partial}{\partial \theta}\right)^2 \\ &= \sin^2\theta \frac{\partial^2}{\partial r^2} + 2\left(\frac{\sin\theta\cos\theta}{r}\right)\frac{\partial^2}{\partial r \partial\theta} + \frac{\cos^2\theta}{r^2}\frac{\partial^2}{\partial\theta^2} - 2\left(\frac{\sin\theta\cos\theta}{r^2}\right)\frac{\partial}{\partial\theta} + \frac{\cos^2\theta}{r}\frac{\partial}{\partial r}.\end{aligned}$$

These combine to give

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}.$$

We will use this in the next section to compute an explicit formula for solving Laplace's equation in the disc.

5.3.2 Poisson's formula via separation of variables

Let $D = \{\mathbf{x} \,|\, |\mathbf{x}| < a\}$ denote the disc of radius $a > 0$. We wish to solve the boundary-value problem

$$\begin{cases} \Delta u = 0 & \text{in } D, \text{ and} \\ u = \tilde{h} & \text{on } \partial D, \end{cases} \tag{5.3}$$

We will write u in polar coordinates, so Laplace's equation becomes

$$\frac{\partial^2 u}{\partial r^2}(r,\theta) + \frac{1}{r}\frac{\partial u}{\partial r}(r,\theta) + \frac{1}{r^2}\frac{\partial^2 u}{\partial\theta^2}(r,\theta) = 0$$

for $0 < r < a$ and $\theta \in [0, 2\pi)$, and denote the parametrisation of the boundary data $\tilde{h}$ as h, so $u(a,\theta) = h(\theta) := \tilde{h}(a,\theta)$ (with $\tilde{h}$ expressed in polar coordinates).

We will search for solutions of the form $u(r,\theta) = R(r)\Theta(\theta)$, a technique which is called *separation of variables* and is something we will use several times in the course. The equation becomes

$$R''\Theta + \frac{1}{r}R'\Theta + \frac{1}{r^2}R\Theta'' = 0$$

Multiplying by $r^2/R\Theta$, we have

$$\frac{r^2 R''}{R} + \frac{rR'}{R} + \frac{\Theta''}{\Theta} = 0.$$

Observe that the first and second terms only depend on r and the third term only on θ. Consequently (why?) we obtain two separate ODEs:

$$\Theta'' + \lambda\Theta = 0 \quad \text{and} \quad r^2R'' + rR' - \lambda R = 0,$$

for $\lambda \in \mathbf{R}$. These can be easily solved. We must ensure that Θ is periodic: $\Theta(\theta + 2\pi) = \Theta(\theta)$ for $\theta \in \mathbf{R}$. Thus

$$\lambda = m^2 \quad \text{and} \quad \Theta(\theta) = A_m\cos(m\theta) + B_m\sin(m\theta) \quad (m = 0, 1, 2, \dots).$$

for $A_m, B_m \in \mathbf{R}$. The equation for R is of Euler type, so we can search for solutions of the form $R(r) = r^\alpha$. Substituting this ansatz and $\lambda = m^2$ into the equation for R we find that $\alpha = \pm m$ and

$$R(r) = C_m r^m + D_m r^{-m} \quad (m = 1, 2, 3, \dots) \quad \text{and} \quad R(r) = C_0 + D_0 \ln r \quad (m = 0)$$

for $C_m, D_m \in \mathbf{R}$. (To find the logarithmic solution requires a little more work.)

It seems unreasonable to allow solutions which are not continuous near the origin, so we reject these, which amounts to taking $D_m = 0$ for all $m = 0, 1, 2, \ldots$. Thus we are left with a number of possible solutions $u(r, \theta) = R(r)\Theta(\theta)$ indexed by a non-negative integer m:

$$C_m r^m (A_m \cos(m\theta) + B_m \sin(m\theta)) \quad (m = 0, 1, 2, \ldots).$$

It is of course redundant to have the products $C_m A_m$ and $C_m B_m$ of two constants in each term, so we set $C_m = 1$ for $m > 0$ and $C_0 = 1/2$. Why we make this specific choice will become clear when we choose A_m and B_m. Finally, in order to build a solution that matches the boundary condition from (5.3), $u = \tilde{h}$ on ∂D, we consider linear combinations of these solutions:

$$u(r, \theta) = \frac{1}{2} A_0 + \sum_{m=1}^{\infty} r^m (A_m \cos(m\theta) + B_m \sin(m\theta)) \tag{5.4}$$

The boundary condition can thus be rewritten as

$$h(\theta) = \frac{1}{2} A_0 + \sum_{m=1}^{\infty} a^m (A_m \cos(m\theta) + B_m \sin(m\theta)),$$

which is exactly the Fourier series of h. Thus we choose A_m and B_m to be the Fourier coefficients of h:

$$A_m = \frac{1}{\pi a^m} \int_0^{2\pi} h(\phi) \cos(m\phi) d\phi \quad \text{and} \quad B_m = \frac{1}{\pi a^m} \int_0^{2\pi} h(\phi) \sin(m\phi) d\phi. \tag{5.5}$$

So we have found a representation, (5.4) and (5.5), of a solution to (5.3) provided the Fourier series of h converges to h. However, we can significantly simplify the representation.

Substituting (5.5) in (5.4) we find that

$$\begin{aligned} u(r, \theta) &= \int_0^{2\pi} h(\phi) \frac{d\phi}{2\pi} + \sum_{m=1}^{\infty} \frac{r^m}{\pi a^m} \int_0^{2\pi} h(\phi) \left(\cos(m\phi) \cos(m\theta) + \sin(m\phi) \sin(m\theta) \right) d\phi \\ &= \int_0^{2\pi} h(\phi) \left(1 + 2 \sum_{m=1}^{\infty} \left(\frac{r}{a} \right)^m \cos(m(\theta - \phi)) \right) \frac{d\phi}{2\pi}. \end{aligned}$$

But

$$\begin{aligned} \left(1 + 2 \sum_{m=1}^{\infty} \left(\frac{r}{a} \right)^m \cos(m(\theta - \phi)) \right) &= 1 + \sum_{m=1}^{\infty} \left(\frac{r}{a} \right)^m e^{im(\theta - \phi)} + \sum_{m=1}^{\infty} \left(\frac{r}{a} \right)^m e^{-im(\theta - \phi)} \\ &= 1 + \frac{r e^{i(\theta - \phi)}}{a - r e^{i(\theta - \phi)}} + \frac{r e^{-i(\theta - \phi)}}{a - r e^{-i(\theta - \phi)}} \\ &= \frac{a^2 - r^2}{a^2 - 2ar \cos(\theta - \phi) + r^2}. \end{aligned}$$

Thus, our formula becomes

$$u(r, \theta) = \frac{(a^2 - r^2)}{2\pi} \int_0^{2\pi} \frac{h(\phi)}{a^2 - 2ar \cos(\theta - \phi) + r^2} d\phi. \tag{5.6}$$

This, in turn, can be simplified to

$$u(\mathbf{x}) = \frac{(a^2 - |\mathbf{x}|^2)}{2\pi a} \int_{|\mathbf{y}| = a} \frac{\tilde{h}(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|^2} d\sigma(\mathbf{y}), \tag{5.7}$$

where $d\sigma(\mathbf{y}) = a d\phi$ is arc-length measure and $\tilde{h}(\mathbf{y}) = h(\phi)$ for $\mathbf{y} = (a \cos \phi, a \sin \phi)$. (See homework exercise 3.1.) Formulae (5.6) and (5.7) are two different forms of what is called the *Poisson formula* for the solution to (5.3). The kernel

$$K(\mathbf{x}, \mathbf{y}) = \frac{(|\mathbf{y}|^2 - |\mathbf{x}|^2)}{2\pi |\mathbf{y}|} \frac{1}{|\mathbf{x} - \mathbf{y}|^2}$$

is called the *Poisson kernel* for the disc of radius a.

In our derivation of the Poisson formula, we assumed that the Fourier series of h converged to h. However, formulae (5.6) and (5.7) can be shown to solve (5.3) when h is just continuous. (Recall that there exist continuous functions for which the Fourier series diverges at a point, and thus does not converge to the function.) We will not prove this last step, but just state it as a theorem.

Theorem 5.2. *Let $D = \{\mathbf{x} \,|\, |\mathbf{x}| < a\}$ be the disc of radius a and let $\tilde{h}\colon \partial D \to \mathbf{R}$ be a continuous function. Then there exists a unique continuous function $u\colon \overline{D} \to \mathbf{R}$ which solves* (5.3)*. This function u is smooth in D (see Lemma 5.5 below) and given by* (5.7) *(or equally by* (5.6) *in polar coordinates, with $h(\theta) = \tilde{h}(a\cos\theta, a\sin\theta)$).*

5.3.3 Mean Value Property and the Strong Maximum Principle

Poisson's formula has the following applications.

Theorem 5.3 (Mean Value Property in $\mathbf{R}^2$)**.** *Let $\Omega \subset \mathbf{R}^2$ be an open set and $u\colon \Omega \to \mathbf{R}$ harmonic. Then for any disc $D_a(\mathbf{x}) = \{\mathbf{y} \in \mathbf{R}^2 \,|\, |\mathbf{y} - \mathbf{x}| < a\}$ such that $\overline{D} \subset \Omega$ we have that*

$$u(\mathbf{x}) = \frac{1}{2\pi a} \int_{\partial D_a(\mathbf{x})} u(\mathbf{y}) d\sigma(\mathbf{y}).$$

That is, the value of u at the centre of a disc is equal to the mean value of u over the boundary of the disc.

Proof. By a change of variables and homework exercise 2.4, it suffices to prove the theorem when $\mathbf{x} = \mathbf{0}$ is the origin and so $D_a(\mathbf{x}) = D$ from (5.3). We define a function $\tilde{h}\colon \partial D \to \mathbf{R}$ by $\tilde{h}(\mathbf{y}) = u(\mathbf{y})$ for $\mathbf{y} \in \partial D$. Since we proved there is only one continuous solution to (5.3), we know u is given by (5.7) in D. Thus, in particular,

$$\begin{aligned} u(\mathbf{0}) &= \frac{(a^2 - |\mathbf{0}|^2)}{2\pi a} \int_{|\mathbf{y}|=a} \frac{\tilde{h}(\mathbf{y})}{|\mathbf{0} - \mathbf{y}|^2} d\sigma(\mathbf{y}) \\ &= \frac{a^2}{2\pi a} \int_{|\mathbf{y}|=a} \frac{u(\mathbf{y})}{a^2} d\sigma(\mathbf{y}) \\ &= \frac{1}{2\pi a} \int_{\partial B_a(\mathbf{0})} u(\mathbf{y}) d\sigma(\mathbf{y}) \end{aligned}$$

□

The Mean Value Theorem confirms something we would expect from the physical situations harmonic functions represent. It also has the following corollary. Recall that a set $\Omega \subset \mathbf{R}^n$ is *(path) connected* if for every pair of points $\mathbf{x}, \mathbf{y} \in D$, there exists a continuous function $\gamma\colon [0,1] \to D$ such that $\gamma(0) = \mathbf{x}$ and $\gamma(1) = \mathbf{y}$.

Corollary 5.4 (Strong Maximum Principle in $\mathbf{R}^2$)**.** *Let $\Omega \subset \mathbf{R}^2$ be a connected bounded open set. Let $u\colon \overline{\Omega} \to \mathbf{R}$ be a continuous function which is harmonic in Ω. Then if the maximum or minimum values of u are attained in Ω, then u is a constant function.*

Proof. Suppose the maximum M is attained at a point $\mathbf{x} \in \Omega$, so $u(\mathbf{x}) = M$, and that u is not constant, so there exists a $\mathbf{y} \in \overline{\Omega}$ such that $u(\mathbf{y}) < M$. In fact, because u is continuous, we can assume $\mathbf{y} \in \Omega$. Since Ω is connected, there exists a curve in Ω from $\mathbf{x}$ to $\mathbf{y}$ (see Figure 4). Since u is continuous, there exists a point $\mathbf{z}$ furthest along the curve towards $\mathbf{y}$ such that $u(\mathbf{z}) = M$. Since Ω is open, we can find a sufficiently small $a > 0$ such that $\overline{D_a(\mathbf{z})} \subset \Omega$. By the Mean Value Property,

$$M = u(\mathbf{z}) = \frac{1}{2\pi a} \int_{\partial D_a(\mathbf{z})} u(\mathbf{w}) d\sigma(\mathbf{w}).$$

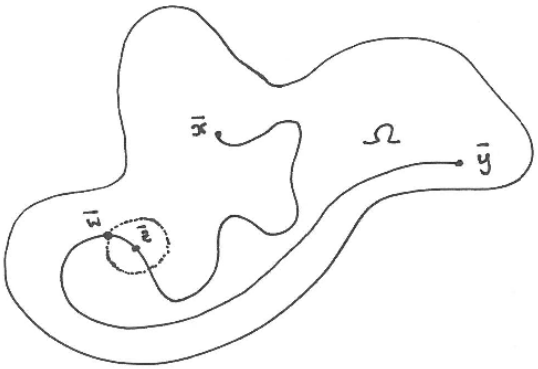


Figure 4: The existence of $\mathbf{w}$ contradicts the fact $\mathbf{z}$ is taken to be the last point along the curve which attains the maximum value M.

Therefore, since $u(\mathbf{w}) \leq M$, we must have $u(\mathbf{w}) = M$ for all $\mathbf{w} \in \partial D_a(\mathbf{z})$, in particular we can find a $\mathbf{w}$ further along the curve such that $u(\mathbf{w}) = M$. This contradicts the fact $\mathbf{z}$ was the last such point.

Therefore, either the maximum is not attained in Ω or u is constant. A similar argument proves the statement for the minimum value. □

Lemma 5.5. *Let $\Omega \subset \mathbf{R}^2$ be an open set and $u\colon \Omega \to \mathbf{R}$ harmonic. Then u possesses all partial derivatives of all orders (such a function is called* smooth*).*

Proof. By a change of variables and homework exercise 2.4, we may assume $\mathbf{0} \in \Omega$ and it suffices to prove u has all partial derivatives at the origin $\mathbf{0}$. Using the Poisson formula, we have an formula for u in a neighbourhood of the origin and it is easy to check this formula can be differentiated as many times as we wish. □

5.4 Laplace's equation in n dimensions

5.4.1 Green's first identity

Suppose $\Omega \subset \mathbf{R}^n$ is an open set with a C^1-boundary.[2] Suppose further that we have two functions $u \in C^2(\overline{\Omega})$ and $v \in C^1(\overline{\Omega})$. The product rule tells us that

$$\partial_j(v\partial_j u) = \partial v_j \partial u_j + v\partial_j^2 u$$

for each $j = 1, 2, \ldots, n$. So

$$\nabla \cdot (v\nabla u) = \nabla v \cdot \nabla u + v\Delta u.$$

Integrating over Ω and applying the divergence theorem, we find

$$\int_{\partial\Omega} v\frac{\partial u}{\partial \mathbf{n}} d\sigma = \int_\Omega (\nabla v \cdot \nabla u + v\Delta u) dV, \tag{5.8}$$

where $\partial u/\partial \mathbf{n} = \mathbf{n} \cdot \nabla u$ and $\mathbf{n}$ is the outward unit normal to $\partial\Omega$. Equation (5.8) is called *Green's first identity.*

[2]This means that $\partial\Omega$ can be written as the union of a finite number of sets, each of which is the graph of a C^1 function with respect to a choice of coordinates. More precisely, there exist a positive integer N such that for each $i = 1, 2, \ldots, N$ there exists an open set $U_i \subset \mathbf{R}^{n-1}$, a matrix A_i whose rows form an orthonormal basis for $\mathbf{R}^n$, and a C^1 function f_i such that $\partial\Omega = \{\mathbf{y} \in \mathbf{R}^n \mid \mathbf{y} = (\mathbf{x}, f_i(\mathbf{x}))A_i \text{ for some } i \text{ and } \mathbf{x} \in U_i\}$

5.4.2 Mean Value Property and the Strong Maximum Principle

We have the following applications of Green's first identity (5.8), which generalise the results we proved earlier when $n = 2$. Observe that we are required to strengthen our assumptions on u, as we have not proved that a harmonic function of more than two variables is smooth (see Lemma 5.5 for the two dimensional result). However, by being careful about how we apply Green's first identity, we can avoid the need to assume $\partial\Omega$ in the statements below is C^1.

Theorem 5.6 (Mean Value Property in $\mathbf{R}^n$, $n \in \mathbf{N}$)**.** *Let $\Omega \subset \mathbf{R}^n$ be an open set and let $u\colon \Omega \to \mathbf{R}$ be a C^2 harmonic function. Then for any ball $B_a(\mathbf{x}) = \{\mathbf{y} \in \mathbf{R}^n \mid |\mathbf{y} - \mathbf{x}| < a\}$ such that $\overline{B_a(\mathbf{x})} \subset \Omega$ we have that*

$$u(\mathbf{x}) = \frac{1}{\omega_{n-1}a^{n-1}} \int_{\partial B_a(\mathbf{x})} u(\mathbf{y}) d\sigma(\mathbf{y}).$$

That is, the value of u at the centre of a ball is equal to the mean value of u over the boundary of the ball.

Proof. We can apply Green's first identity to the functions u as in the statement of the theorem, $v \equiv 1$ and $\Omega = B_a(\mathbf{x})$. We find that

$$\int_{\partial B_a(\mathbf{x})} \frac{\partial u(\mathbf{y})}{\partial \mathbf{n}} d\sigma(\mathbf{y}) = 0.$$

Dividing by the area of $\partial B_a(\mathbf{x})$, which is a constant ω_{n-1} times a^{n-1}, we have

$$\begin{aligned} 0 &= \frac{1}{\omega_{n-1}a^{n-1}} \int_{\partial B_a(\mathbf{x})} \frac{\partial u(\mathbf{y})}{\partial \mathbf{n}} d\sigma(\mathbf{y}) = \frac{1}{\omega_{n-1}} \int_{\partial B_1(\mathbf{0})} \mathbf{z} \cdot \nabla u(\mathbf{x} + a\mathbf{z}) d\sigma(\mathbf{z}) = \frac{1}{\omega_{n-1}} \int_{\partial B_1(\mathbf{0})} \frac{\partial u(\mathbf{x} + a\mathbf{z})}{\partial a} d\sigma(\mathbf{z}) \\ &= \frac{1}{\omega_{n-1}} \frac{d}{da} \int_{\partial B_1(\mathbf{0})} u(\mathbf{x} + a\mathbf{z}) d\sigma(\mathbf{z}) = \frac{d}{da} \left(\frac{1}{\omega_{n-1}a^{n-1}} \int_{\partial B_a(\mathbf{x})} u(\mathbf{y}) d\sigma(\mathbf{y}) \right). \end{aligned}$$

Thus, the quantity in parenthesis on the right-hand side above is constant. Taking the limit $a \to 0$ we see that this constant must be $u(\mathbf{x})$, which proves the theorem. □

Once again, we can use the mean value property to prove a maximum principle.

Corollary 5.7 (Strong Maximum Principle in $\mathbf{R}^n$, $n \in \mathbf{N}$)**.** *Let $\Omega \subset \mathbf{R}^n$ be a connected bounded open set. Let $u\colon \overline{\Omega} \to \mathbf{R}$ be a continuous function which is of class C^2 and harmonic in Ω. If the maximum or minimum values of u are attained in Ω, then u is a constant function.*

Proof. The proof of this is identical to that of Corollary 5.4. □

5.4.3 Dirichlet's Principle

We can now demonstrate an important idea which connects harmonic functions to a notion of energy (borrowed directly from physics). It states that amongst all (reasonably smooth) functions $w\colon \overline{\Omega} \to \mathbf{R}$ with a given boundary value $w = h$ on $\partial\Omega$, a function u which solves

$$\begin{cases} \Delta u = 0 & \text{in } \Omega, \text{ and} \\ u = h & \text{on } \partial\Omega, \end{cases} \tag{5.9}$$

should minimise some sort of 'energy'. We now state this idea more precisely.

Theorem 5.8. *Suppose that $\Omega \subset \mathbf{R}^n$ is a connected bounded open set with a C^1 boundary $\partial\Omega$ and h is a C^1 function defined on $\partial\Omega$. For any C^1 function $w\colon \overline{\Omega} \to \mathbf{R}$ such that $w(\mathbf{x}) = h(\mathbf{x})$ for all $\mathbf{x} \in \partial\Omega$, define*

$$E[w] = \frac{1}{2} \int_\Omega |\nabla w|^2.$$

Then a solution $u \in C^1(\overline{\Omega})$ to (5.9) which is C^2 in Ω is such that

$$E[u] \leq E[w]$$

for any w as above.

Proof. Given u and w as above, observe that $v := w - u$ is such that $v(\mathbf{x}) = 0$ for all $\mathbf{x} \in \partial\Omega$. We can then compute

$$2E[w] = \int_\Omega |\nabla v + \nabla u|^2 = \int_\Omega (|\nabla v|^2 + |\nabla u|^2 + 2\nabla v \cdot \nabla u) = \left(\int_\Omega |\nabla v|^2\right) + 2E[u] + 2\int_\Omega \nabla v \cdot \nabla u.$$

Applying Green's first identity (5.8), we see that

$$\int_\Omega \nabla v \cdot \nabla u = \int_{\partial\Omega} v \frac{\partial u}{\partial \mathbf{n}} d\sigma - \int_\Omega v \Delta u = 0.$$

Thus $E[w] \geq E[u]$ since $\int_\Omega |\nabla v|^2 \geq 0$. □

5.4.4 Green's second identity and the fundamental solution

In homework exercise 4.1 we used Green's first identity (5.8) to prove Green's second identity: *Green's second identity* states that for two functions $u, v \in C^2(\overline{\Omega})$

$$\int_\Omega u(\mathbf{x})\Delta v(\mathbf{x}) - v(\mathbf{x})\Delta u(\mathbf{x}) d\mathbf{x} = \int_{\partial\Omega} u(\mathbf{x}) \frac{\partial v}{\partial \mathbf{n}}(\mathbf{x}) - v(\mathbf{x}) \frac{\partial u}{\partial \mathbf{n}}(\mathbf{x}) d\sigma(\mathbf{x}). \tag{5.10}$$

We also considered the function $\Phi\colon \mathbf{R}^n \setminus \{\mathbf{0}\} \to \mathbf{R}$ defined by

$$\Phi(\mathbf{x}) = \begin{cases} -\frac{1}{2\alpha(2)} \ln|\mathbf{x}| & \text{if } n = 2, \\ \frac{1}{n(n-2)\alpha(n)} \frac{1}{|\mathbf{x}|^{n-2}} & \text{if } n > 2, \end{cases} \tag{5.11}$$

where $\alpha(n)$ is the volume of the unit ball in $\mathbf{R}^n$. The function Φ is called the *fundamental solution* of the Laplace operator. We proved Φ was harmonic in $\mathbf{R}^n \setminus \{\mathbf{0}\}$ and the outward normal derivative of Φ on the boundary of the domain $B_r(\mathbf{0}) := \{\mathbf{y} \in \mathbf{R}^n \mid |\mathbf{y}| < r\}$ is

$$\frac{\partial \Phi}{\partial \mathbf{n}}(\mathbf{x}) = \frac{-1}{n\alpha(n)} \frac{1}{|\mathbf{x}|^{n-1}} \tag{5.12}$$

for all $x \in \partial B_r(\mathbf{0})$ and each $n = 2, 3, \ldots$ (homework exercise 6.1).

We can use these facts to prove the following lemma.

Lemma 5.9. *Let Ω be an open bounded set with C^1 boundary and suppose that $u \in C^2(\overline{\Omega})$ is harmonic in Ω. Then*

$$u(\mathbf{x}) = \int_{\partial\Omega} \left\{ \Phi(\mathbf{y} - \mathbf{x}) \left(\frac{\partial u}{\partial \mathbf{n}}\right)(\mathbf{y}) - \left(\frac{\partial \Phi}{\partial \mathbf{n}}\right)(\mathbf{y} - \mathbf{x}) u(\mathbf{y}) \right\} d\sigma(\mathbf{y}). \tag{5.13}$$

for each $\mathbf{x} \in \Omega$

Proof. We wish to apply Green's second identity (5.10) to the functions $\Phi(\cdot - \mathbf{x})$ and u in Ω. However we cannot as $\Phi(\cdot - \mathbf{x})$ is not defined at $\mathbf{x}$. We instead apply (5.10) to $\Omega_r := \Omega \setminus \overline{B_r(\mathbf{x})}$. We obtain

$$0 = \int_{\partial\Omega_r} \left\{ \Phi(\mathbf{y} - \mathbf{x}) \left(\frac{\partial u}{\partial \mathbf{n}}\right)(\mathbf{y}) - \left(\frac{\partial \Phi}{\partial \mathbf{n}}\right)(\mathbf{y} - \mathbf{x}) u(\mathbf{y}) \right\} d\sigma(\mathbf{y}).$$

However, $\partial\Omega_r$ has two components, $\partial\Omega$ and $\partial B_r(\mathbf{x})$. The integral over $\partial\Omega$ is exactly the right-hand side of (5.13), so we only need to calculate the integral over $\partial B_r(\mathbf{x})$. From (5.11) it is clear that Φ is a radial function—that is, we can write $\Phi(\mathbf{x}) = \phi(|\mathbf{x}|)$ for

$$\phi(r) = \begin{cases} -\frac{1}{2\alpha(2)} \ln|r| & \text{if } n = 2, \\ \frac{1}{n(n-2)\alpha(n)} \frac{1}{r^{n-2}} & \text{if } n > 2. \end{cases}$$

Remembering that the outward normal $\mathbf{n}$ to Ω_r is actually an inward normal to $B_r(\mathbf{x})$ on $\partial B_r(\mathbf{x})$, we have from (5.12) that

$$\frac{\partial \Phi}{\partial \mathbf{n}}(\mathbf{y} - \mathbf{x}) = \frac{1}{n\alpha(n)} \frac{1}{r^{n-1}}.$$

Thus

$$\begin{aligned}
&\int_{\partial B_r(\mathbf{x})} \left\{ \Phi(\mathbf{y}-\mathbf{x}) \left(\frac{\partial u}{\partial \mathbf{n}}\right)(\mathbf{y}) - \left(\frac{\partial \Phi}{\partial \mathbf{n}}\right)(\mathbf{y}-\mathbf{x}) u(\mathbf{y}) \right\} d\sigma(\mathbf{y}) \\
=&\int_{\partial B_r(\mathbf{x})} \phi(r) \left(\frac{\partial u}{\partial \mathbf{n}}\right)(\mathbf{y}) d\sigma(\mathbf{y}) - \int_{\partial B_r(\mathbf{x})} \frac{1}{n\alpha(n)} \frac{1}{r^{n-1}} u(\mathbf{y}) d\sigma(\mathbf{y}) \\
=&\phi(r) \left(\int_{\partial B_r(\mathbf{x})} \left(\frac{\partial u}{\partial \mathbf{n}}\right)(\mathbf{y}) d\sigma(\mathbf{y}) \right) - \left(\frac{1}{n\alpha(n) r^{n-1}} \int_{\partial B_r(\mathbf{x})} u(\mathbf{y}) d\sigma(\mathbf{y}) \right).
\end{aligned}$$

Applying the divergence theorem (with $-\mathbf{n}$ being the outward unit normal), we see that

$$\left(\int_{\partial B_r(\mathbf{x})} \left(\frac{\partial u}{\partial \mathbf{n}}\right)(\mathbf{y}) d\sigma(\mathbf{y}) \right) = -\int_{B_r(\mathbf{x})} \Delta u(\mathbf{y}) d\mathbf{y} = 0.$$

Since $n\alpha(n) r^{n-1}$ is the surface area of $\partial B_r(\mathbf{x})$,[3] the mean value property (Lemma 5.6) says

$$\left(\frac{1}{n\alpha(n) r^{n-1}} \int_{\partial B_r(\mathbf{x})} u(\mathbf{y}) d\sigma(\mathbf{y}) \right) = u(\mathbf{x}).$$

Putting these facts together, we see the lemma is proved. □

5.4.5 Green's functions

At first sight (5.13) appears to be a useful formula, as it expresses a harmonic function in a domain Ω in terms of its behaviour on the boundary $\partial\Omega$. However, physically we do not expect to have to specify both the value of u and the value of $\partial u/\partial \mathbf{n}$ on the boundary. Therefore we wish to modify the fundamental solution (5.11) somewhat to eliminate one of the terms in (5.13).

To be more precise, suppose we wanted to solve the same boundary value problem we considered in Section 5.4.3:

$$\begin{cases} \Delta u = 0 & \text{in } \Omega, \text{ and} \\ u = h & \text{on } \partial\Omega. \end{cases} \tag{5.9}$$

If we can find a modification G of Φ which has very similar properties to Φ but is also zero on the boundary, then we should be able to solve (5.9) via a formula like (5.13).

We now make this ideas more precise.

Definition 5.10. *Let $\Omega \subset \mathbf{R}^n$ be an open bounded set with C^1 boundary. A function $G\colon \Omega \times \Omega \to \mathbf{R}$ is called a* Green's function *for the Laplacian in Ω if:*

1. *the function $\mathbf{y} \mapsto G(\mathbf{x}, \mathbf{y})$ belongs to $C^2(\overline{\Omega} \setminus \{\mathbf{x}\})$ and is harmonic for $\mathbf{y} \neq \mathbf{x}$;*
2. *$G(\mathbf{x}, \mathbf{y}) = 0$ for all $\mathbf{y} \in \partial\Omega$ and $\mathbf{x} \in \Omega$;*
3. *for each $\mathbf{x} \in \Omega$, the function $\mathbf{y} \mapsto G(\mathbf{x}, \mathbf{y}) - \Phi(\mathbf{y} - \mathbf{x})$ has a continuous extension which belongs to $C^2(\overline{\Omega})$ and is harmonic in Ω.*

By section 5.2, we already know any solution u to (5.9) is unique. The following theorem transforms the problem of proving the existence of solutions to (5.9) to that of proving the existence of a Green's function.

Theorem 5.11. *Let $\Omega \subset \mathbf{R}^n$ be an open bounded set with C^2 boundary and suppose $h \in C^2(\partial\Omega)$.[4] If there exists a Green's function G for the Laplacian in Ω then there exists (a unique) solution of (5.9). This solution is given by the formula*

$$u(\mathbf{x}) = -\int_{\partial\Omega} \left(\frac{\partial G(\mathbf{x}, \cdot)}{\partial \mathbf{n}}(\mathbf{y}) \right) h(\mathbf{y}) d\sigma(\mathbf{y}). \tag{5.14}$$

where $(\partial G(\mathbf{x}, \cdot)/\partial \mathbf{n})(\mathbf{y}) := \mathbf{n}(\mathbf{y}) \cdot \nabla_{\mathbf{y}} G(\mathbf{x}, \mathbf{y})$ is the normal derivative of $\mathbf{y} \mapsto G(\mathbf{x}, \mathbf{y})$.

[3] Prove this!

[4] If we look back at how we proved Green's identities, it is clear that in fact we only need to assume Ω has a C^1 boundary and $h \in C^1(\partial\Omega)$.

Proof. Apply Green's second identity (5.10) to the functions u and $\mathbf{y} \mapsto G(\mathbf{x}, \mathbf{y}) - \Phi(\mathbf{y} - \mathbf{x})$ and add the result to (5.13). □

Theorem 5.12. *Let $\Omega \subset \mathbf{R}^n$ be an open bounded set with C^2 boundary.*

1. *There exists at most one Green's function for the Laplacian in Ω.*
2. *$G(\mathbf{x}, \mathbf{y}) = G(\mathbf{y}, \mathbf{x})$ for all $\mathbf{x}, \mathbf{y} \in \Omega$.*

Proof. See homework exercise 6.4. □

5.4.6 Finding the Green's function: the example of the upper half-plane

Let us now take a concrete example and calculate the Green's function. We will consider the upper half-plane $\mathbf{R}^n_+$. You will notice immediately that $\mathbf{R}^n_+$ is not bounded, so does not fit into the theory we have discussed so far. But the ideas we will discuss are a little simpler in $\mathbf{R}^n_+$, so it is a good example to study. Once we have derived our formula, we will prove rigorously that it is does what we hope.

Observe that property 3 of Definition 5.10 requires that for each fixed $\mathbf{x} \in \mathbf{R}^n_+$ the function $\mathbf{y} \mapsto v_{\mathbf{x}}(\mathbf{y}) := G(\mathbf{x}, \mathbf{y}) - \Phi(\mathbf{y} - \mathbf{x})$ is harmonic in $\mathbf{R}^n_+$. We can also see from property 2 that

$$v_{\mathbf{x}}(\mathbf{y}) := G(\mathbf{x}, \mathbf{y}) - \Phi(\mathbf{y} - \mathbf{x}) = -\Phi(\mathbf{y} - \mathbf{x}) \quad \text{for } \mathbf{y} \in \mathbf{R}^n_+.$$

Whence, $v_{\mathbf{x}}$ is a solution to the boundary value problem

$$\begin{cases} \Delta v_{\mathbf{x}} = 0 & \text{in } \mathbf{R}^n_+, \text{ and} \\ v_{\mathbf{x}} = -\Phi(\cdot - \mathbf{x}) & \text{on } \partial\mathbf{R}^n_+. \end{cases} \tag{5.15}$$

However, we can use the symmetry of the domain $\mathbf{R}^n_+$ and of Φ to find a solution to (5.15). For $\mathbf{x} = (x_1, x_2, \ldots, x_{n-1}, x_n)$ define $\tilde{\mathbf{x}} = (x_1, x_2, \ldots, x_{n-1}, -x_n)$ to be the reflection in the plane $\partial\mathbf{R}^n_+$ (see Figure 5). Then, for $\mathbf{y} \in \partial\mathbf{R}^n_+$, we have $|\mathbf{y} - \mathbf{x}| = |\mathbf{y} - \tilde{\mathbf{x}}|$, and since Φ is a radial function $\Phi(\mathbf{y} - \mathbf{x}) = \Phi(\mathbf{y} - \tilde{\mathbf{x}})$. Moreover, since $\tilde{\mathbf{x}} \notin \mathbf{R}^n_+$, $\mathbf{y} \mapsto \Phi(\mathbf{y} - \tilde{\mathbf{x}})$ is harmonic in $\mathbf{R}^n_+$. That is, the solution to (5.15) is $v_{\mathbf{y}}(\mathbf{x}) = -\Phi(\mathbf{y} - \tilde{\mathbf{x}})$. Which means the Green's function for $\mathbf{R}^n_+$ is

$$G(\mathbf{x}, \mathbf{y}) = \Phi(\mathbf{y} - \mathbf{x}) - \Phi(\mathbf{y} - \tilde{\mathbf{x}}) \tag{5.16}$$

In order to make use of (5.14), we need to compute $\frac{\partial G(\mathbf{x}, \cdot)}{\partial \mathbf{n}}$. We can easily check that

$$\frac{\partial G(\mathbf{x}, \mathbf{y})}{\partial y_n} = \frac{1}{n\alpha(n)} \frac{(y_n - x_n)}{|\mathbf{y} - \mathbf{x}|^n} - \frac{1}{n\alpha(n)} \frac{(y_n + x_n)}{|\mathbf{y} - \tilde{\mathbf{x}}|^n}$$

and since the outward unit normal to $\partial\mathbf{R}^n_+$ is $\mathbf{n} = (0, 0, \ldots, 0, -1)$, for $\mathbf{y} \in \partial\mathbf{R}^n_+$ we have

$$\frac{\partial G(\mathbf{x}, \cdot)}{\partial \mathbf{n}}(\mathbf{y}) = -\frac{2x_n}{n\alpha(n)} \frac{1}{|\mathbf{x} - \mathbf{y}|^n}.$$

Thus, we expect

$$u(\mathbf{x}) = \begin{cases} \int_{\partial\mathbf{R}^n_+} \frac{2x_n}{n\alpha(n)} \frac{1}{|\mathbf{x}-\mathbf{y}|^n} h(\mathbf{y}) d\sigma(\mathbf{y}) & \text{if } \mathbf{x} \in \mathbf{R}^n_+; \\ h(\mathbf{x}) & \text{if } \mathbf{x} \in \partial\mathbf{R}^n_+. \end{cases} \tag{5.17}$$

to solve (5.9). As we said, we cannot apply Theorem 5.11 on an unbounded domain, but our next theorem proves that (5.17) does indeed provide a solution to (5.9).

Theorem 5.13. *Suppose $h \in C(\partial\mathbf{R}^n_+)$ is a bounded function. Then $u \colon \overline{\mathbf{R}^n_+} \to \mathbf{R}$ defined by (5.17) is a continuous function in $\overline{\mathbf{R}^n_+}$ and solves (5.9) with $\Omega = \mathbf{R}^n_+$. Moreover, if there exists an $R > 0$ such that $h(\mathbf{y}) = 0$ when $|\mathbf{y}| > R$, then (5.17) is the only solution to (5.9) such that $u(\mathbf{x}) \to 0$ as $|\mathbf{x}| \to \infty$.*

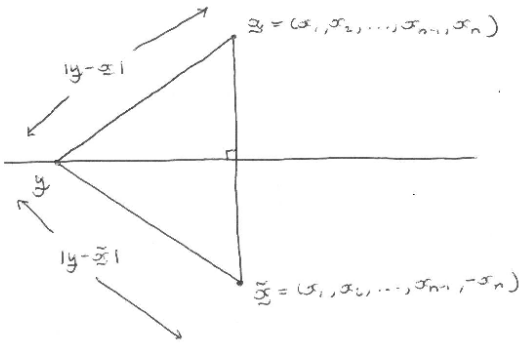


Figure 5: The point $\tilde{\mathbf{x}}$ is the mirror image of $\mathbf{x}$ in the hyperplane $\partial\mathbf{R}^n_+$.

Proof. First, we will show that u defined by (5.17) is harmonic in $\mathbf{R}^n_+$. We know that, for $\mathbf{x} \in \partial\mathbf{R}^n_+$, $\mathbf{y} \mapsto G(\mathbf{x}, \mathbf{y})$ is smooth and harmonic in $\mathbf{R}^n_+$. Because of Theorem 5.12, $G(\mathbf{x}, \mathbf{y}) = G(\mathbf{y}, \mathbf{x})$, so $\mathbf{x} \mapsto G(\mathbf{x}, \mathbf{y})$ and $\mathbf{x} \mapsto \partial_{y_n} G(\mathbf{x}, \mathbf{y}) := K(\mathbf{x}, \mathbf{y})$ is harmonic in $\mathbf{R}^n_+$ for $\mathbf{y} \in \partial\mathbf{R}^n_+$. (This can also be checked by direct calculation.) We can also compute that

$$1 = \int_{\partial\mathbf{R}^n_+} K(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}) \tag{5.18}$$

Since h is bounded and K is smooth, u defined by (5.17) is smooth in $\mathbf{R}^n_+$ and we can interchange differentiation and integration, so

$$\Delta u(x) = \int_{\partial\mathbf{R}^n_+} \Delta_{\mathbf{x}} K(\mathbf{x}, \mathbf{y}) h(\mathbf{y}) d\sigma(\mathbf{y}) = 0.$$

We now need to show that u is continuous, in particular continuous at the boundary $\partial\mathbf{R}^n_+$. Fix $\mathbf{x}^0 \in \partial\mathbf{R}^n_+$ and $\varepsilon > 0$. Since h is continuous we can find a $\delta > 0$ such that

$$|h(\mathbf{y}) - h(\mathbf{x}^0)| < \varepsilon \quad \text{if} \quad |\mathbf{y} - \mathbf{x}^0| < \delta \quad \text{and} \quad \mathbf{y} \in \partial\mathbf{R}^n_+. \tag{5.19}$$

If $|\mathbf{x} - \mathbf{x}^0| < \delta/2$ and $\mathbf{x} \in \mathbf{R}^n_+$, then

$$\begin{aligned} |u(\mathbf{x}) - h(\mathbf{x}^0)| &= \left| \int_{\partial\mathbf{R}^n_+} K(\mathbf{x}, \mathbf{y})(h(\mathbf{y}) - h(\mathbf{x}^0)) d\sigma(\mathbf{y}) \right| \\ &\le \int_{\partial\mathbf{R}^n_+ \cap B_\delta(\mathbf{x}^0)} K(\mathbf{x}, \mathbf{y}) |h(\mathbf{y}) - h(\mathbf{x}^0)| d\sigma(\mathbf{y}) \\ &\quad + \int_{\partial\mathbf{R}^n_+ \setminus B_\delta(\mathbf{x}^0)} K(\mathbf{x}, \mathbf{y})(h(\mathbf{y}) - h(\mathbf{x}^0)) d\sigma(\mathbf{y}) \\ &=: I + J. \end{aligned}$$

Now (5.18) and (5.19) imply

$$I \le \varepsilon \int_{\partial\mathbf{R}^n_+} K(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}) = \varepsilon.$$

Furthermore, if $|\mathbf{x} - \mathbf{x}^0| < \delta/2$ and $\mathbf{y} \in \partial\mathbf{R}^n_+ \setminus B_\delta(\mathbf{x}^0)$, then

$$|\mathbf{y} - \mathbf{x}^0| \le |\mathbf{y} - \mathbf{x}| + |\mathbf{x} - \mathbf{x}^0| \le |\mathbf{y} - \mathbf{x}| + \delta/2 \le |\mathbf{y} - \mathbf{x}| + |\mathbf{y} - \mathbf{x}^0|/2,$$

so $|\mathbf{y} - \mathbf{x}| \ge \frac{1}{2}|\mathbf{y} - \mathbf{x}^0|$. Thus

$$\begin{aligned} J &\le 2\|h\|_{L^\infty} \int_{\partial\mathbf{R}^n_+ \setminus B_\delta(\mathbf{x}^0)} K(\mathbf{x}, \mathbf{y}) d\sigma(\mathbf{y}) \\ &\le \frac{2^{n-2}\|h\|_{L^\infty} x_n}{n\alpha(n)} \int_{\partial\mathbf{R}^n_+ \setminus B_\delta(\mathbf{x}^0)} |\mathbf{y} - \mathbf{x}^0|^{-n} d\sigma(\mathbf{y}) \to 0 \end{aligned}$$

as $x_n \to 0$. Thus, we see that $|u(\mathbf{x}) - h(\mathbf{x}^0)| \leq 2\varepsilon$ provided $|\mathbf{x} - \mathbf{x}^0|$ is sufficiently small.

To prove that (5.17) is the only solution the only solution to (5.9) such that $u(\mathbf{x}) \to 0$ as $|\mathbf{x}| \to \infty$ we may also assume that there exists an $R > 0$ such that $h(\mathbf{y}) = 0$ when $|\mathbf{y}| > R$. Therefore, if $|\mathbf{x}| \geq 2^k R$ for $k \in \mathbf{N}$, then

$$\begin{aligned} |u(\mathbf{x})| &= \left| \int_{\partial \mathbf{R}^n_+} K(\mathbf{x}, \mathbf{y}) h(\mathbf{y}) d\sigma(\mathbf{y}) \right| \\ &\leq \frac{2}{n\alpha(n)} \int_{\partial \mathbf{R}^n_+} |\mathbf{x} - \mathbf{y})|^{1-n} |h(\mathbf{y})| d\sigma(\mathbf{y}) \\ &\leq \frac{2^{-(n-1)k} R^{-(n-1)}}{n\alpha(n)} R^n \|h\|_{L^\infty} = \frac{2^{-(n-1)k} R \|h\|_{L^\infty}}{n\alpha(n)} \end{aligned}$$

Suppose v was a second solution to (5.17) such that $u(\mathbf{x}) \to 0$ as $|\mathbf{x}| \to \infty$. Then $u(\mathbf{y}) - v(\mathbf{y}) = 0$ for $\mathbf{y} \in \partial \mathbf{R}^n_+$. For each $\varepsilon > 0$ we can choose k sufficiently large so that $|u(\mathbf{x})| + |v(\mathbf{x})| \leq \varepsilon$ for $|\mathbf{x}| > 2^k R$. Then by the Weak Maximum Principle (Theorem 5.1), we have that $|u(\mathbf{x}) - v(\mathbf{x})| < \varepsilon$ for $|\mathbf{x}| \leq 2^k R$. Since $\varepsilon > 0$ was arbitrary, we must have $u(\mathbf{x}) = v(\mathbf{x})$. □

5.4.7 Finding the Green's function: the example of the unit ball

We now consider a second concrete example — when our domain is the unit ball

$$B := B_1(\mathbf{0}) = \{\mathbf{x} \in \mathbf{R}^n \colon |\mathbf{x}| < 1\}.$$

The idea is essentially the same as in section 5.4.6, but it is technically harder, as it is not as easy to see exactly how one should 'reflect' the singularity in the funadmental solution. An approach which works is to use the *Kelvin transform* of a point $\mathbf{x} \in \mathbf{R}^n \setminus \{\mathbf{0}\}$ which is defined to be

$$\mathbf{x}^* = \frac{\mathbf{x}}{|\mathbf{x}|^2}$$

Just as in section 5.4.6 property 3 of Definition 5.10 requires that for each fixed $\mathbf{x} \in B$ the function $\mathbf{y} \mapsto v_{\mathbf{x}}(\mathbf{y}) := G(\mathbf{x}, \mathbf{y}) - \Phi(\mathbf{y} - \mathbf{x})$ is harmonic in B. We can also see from property 2 that

$$v_{\mathbf{x}}(\mathbf{y}) := G(\mathbf{x}, \mathbf{y}) - \Phi(\mathbf{y} - \mathbf{x}) = -\Phi(\mathbf{y} - \mathbf{x}) \quad \text{for } \mathbf{y} \in B.$$

Whence, $v_{\mathbf{x}}$ is a solution to the boundary value problem

$$\begin{cases} \Delta v_{\mathbf{x}} = 0 & \text{in } B, \text{ and} \\ v_{\mathbf{x}} = -\Phi(\cdot - \mathbf{x}) & \text{on } \partial B. \end{cases} \tag{5.20}$$

Thus, in order to find the Green's function G for B it sufficies to find $v_{\mathbf{x}}$ for each $\mathbf{x} \in B$. Once again we try to find $v_{\mathbf{x}}$ by considering a transformation of the fundamental solution Φ. First observe that, for $\mathbf{y} \in \partial B$ and $\mathbf{x} \neq \mathbf{0}$,

$$\begin{aligned} |\mathbf{x}|^2 |\mathbf{y} - \mathbf{x}^*|^2 &= |\mathbf{x}|^2 \left(|\mathbf{y}|^2 - 2\mathbf{y} \cdot \mathbf{x}^* + |\mathbf{x}^*|^2 \right) = |\mathbf{x}|^2 \left(|\mathbf{y}|^2 - \frac{2\mathbf{y} \cdot \mathbf{x}}{|\mathbf{x}|^2} + \frac{1}{|\mathbf{x}|^2} \right) \\ &= |\mathbf{x}|^2 - \frac{2\mathbf{y} \cdot \mathbf{x}}{|\mathbf{x}|^2} + 1 = |\mathbf{x}|^2 - \frac{2\mathbf{y} \cdot \mathbf{x}}{|\mathbf{x}|^2} + |\mathbf{y}|^2 \\ &= |\mathbf{x} - \mathbf{y}|^2. \end{aligned}$$

Therefore, because Φ is radial, $-\Phi(|\mathbf{x}|(\mathbf{y} - \mathbf{x}^*)) = -\Phi(\mathbf{x} - \mathbf{y})$ for $\mathbf{y} \in \partial B$ and $\mathbf{x} \in B$. Moreover, $\mathbf{y} \mapsto -\Phi(|\mathbf{x}|(\mathbf{y} - \mathbf{x}^*))$ is harmonic in B. Thus we have identified

$$v_{\mathbf{x}}(\mathbf{y}) = -\Phi(|\mathbf{x}|(\mathbf{y} - \mathbf{x}^*))$$

as the solution to (5.20). Consequently the Green's function for the unit ball is

$$G(\mathbf{x}, \mathbf{y}) = \Phi(\mathbf{y} - \mathbf{x}) - \Phi(|\mathbf{x}|(\mathbf{y} - \mathbf{x}^*). \tag{5.21}$$

Since the unit ball B is an open bounded set with C^2 boundary, we can apply Theorem 5.11 directly to conclude that (5.14) with G as in (5.21) is a solution to (5.9) with $\Omega = B$.

For the sake of completeness we evaliuate $\partial G(\mathbf{x}, \cdot)/\partial \mathbf{n}$ so we can write out (5.14) explicitely. Writing $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ and $\mathbf{y} = (y_1, y_2, \ldots, y_n)$ we have

$$\frac{\partial \Phi}{\partial y_i}(\mathbf{x} - \mathbf{y}) = \frac{1}{n\alpha(n)} \frac{x_i - y_i}{|\mathbf{x} - \mathbf{y}|^n}$$

and

$$\frac{\partial \Phi}{\partial y_i}(|\mathbf{x}|(\mathbf{x} - \mathbf{y})) = \frac{1}{n\alpha(n)} \frac{x_i - |\mathbf{x}|^2 y_i}{|\mathbf{x}||\mathbf{y} - \mathbf{x}^*|^n} = \frac{1}{n\alpha(n)} \frac{x_i - |\mathbf{x}|^2 y_i}{|\mathbf{x} - \mathbf{y}|^n}$$

when $\mathbf{y} \in \partial B$. So, according to (5.21) and the above calulations,

$$\begin{aligned} \frac{\partial G(\mathbf{x}, \cdot)}{\partial \mathbf{n}}(\mathbf{y}) &= \sum_{i=1}^{n} y_i \frac{\partial G(\mathbf{x}, \mathbf{y})}{\partial y_i} \\ &= \frac{1}{n\alpha(n)|\mathbf{x} - \mathbf{y}|^n} \sum_{i=1}^{n} y_i \left((x_i - y_i) - x_i + y_i |\mathbf{x}|^2 \right) \\ &= \frac{|\mathbf{x}|^2 - 1}{n\alpha(n)|\mathbf{x} - \mathbf{y}|^n}, \end{aligned}$$

and we can write the unique solution for (5.9) for $\Omega = B$ as

$$u(\mathbf{x}) = \frac{1 - |\mathbf{x}|^2}{n\alpha(n)} \int_{\partial B} \frac{g(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|^n} d\sigma(y).$$

This formula is called the *Poisson formula* for the unit ball and the function

$$K(\mathbf{x}, \mathbf{y}) := \frac{1 - |\mathbf{x}|^2}{n\alpha(n)|\mathbf{x} - \mathbf{y}|^n}$$

is called the *Poisson kernel* for the unit ball.

6 The wave equation

6.1 One spatial dimension: d'Alembert's formula

We will now consider the wave equation

$$\begin{cases} \partial_t^2 u(x,t) - c^2 \partial_x^2 u(x,t) = 0 & \text{for } x \in \mathbf{R} \text{ and } t > 0, \\ u(x,0) = g(x) \quad \text{and} \quad \partial_t u(x,0) = h(x) & \text{for } x \in \mathbf{R}. \end{cases} \tag{6.1}$$

As we discussed in Section 4.2, physically this is a reasonable initial value problem to try to solve. A helpful property of this equation is that the associated operator factors, so we can rewrite the differential equation in (6.1) as[5]

$$(\partial_t + c\partial_x)(\partial_t - c\partial_x)u(x,t) = 0.$$

This means that finding u solving the differential equation in (6.1) is equivalent to finding u and v solving the system

$$\begin{cases} \partial_t v(x,t) + c\partial_x v(x,t) = 0 \\ \partial_t u(x,t) - c\partial_x u(x,t) = v(x,t) \end{cases} \tag{6.2}$$

We can use the method of characteristics to solve (6.2). Indeed, both equations in (6.2) are of the form of (†) in homework exercise 1.6. Looking at the first equation in (6.2), we need to apply (‡) from Solutions 1 with $n = 1$, $b = c$ and $f(x,t) = 0$. The solution is thus

$$v(x,t) = a(x - ct),$$

[5]These two factors commute, of course, so we could equally write $(\partial_t - c\partial_x)(\partial_t + c\partial_x)u(x,t) = 0$.

for some function a such that $v(x,0) = a(x)$. (Observe, we cannot make use of the initial conditions for u at this point.) Substituting this solution in the second equation in (6.2), we now need to solve

$$\partial_t u(x,t) - c\partial_x u(x,t) = a(x-ct).$$

Applying (‡) from Solutions 1 with $n = 1$, $b = -c$, $f(x,t) = a(x-ct)$ and $g(x) = g(x)$, we see that

$$\begin{aligned} u(x,t) &= g(x+ct) + \int_0^t a((x+cs) - c(t-s))ds = g(x+ct) + \int_0^t a(x-ct+2cs)ds \\ &= g(x+ct) + \frac{1}{2c}\int_{x-ct}^{x+ct} a(y)dy. \end{aligned}$$

Although this is a formula for the solution u, a is still unknown to us. To find out what a is, we need to make use of the initial condition $\partial_t u(x,0) = h(x)$. Differentiating the formula above yields (with the help of the First Fundamental Theorem of Calculus (analysens huvudsats))

$$\partial_t u(x,t) = cg'(x+ct) + \frac{1}{2c}\left(ca(x+ct) + ca(x-ct)\right)$$

and setting $t = 0$ gives $h(x) = \partial_t u(x,0) = cg'(x) + a(x)$, so $a(x) = h(x) - cg'(x)$ and

$$\begin{aligned} u(x,t) &= g(x+ct) + \frac{1}{2c}\int_{x-ct}^{x+ct} h(y) - cg'(y)dy \\ &= \frac{1}{2}\left(g(x+ct) + g(x-ct)\right) + \frac{1}{2c}\int_{x-ct}^{x+ct} h(y)dy. \end{aligned} \tag{6.3}$$

Formula (6.3) is called *d'Alembert's formula*.

Theorem 6.1. *Assume that $g \in C^2(\mathbf{R})$ and $h \in C^1(\mathbf{R})$. Then u defined by* (6.3) *is a $C^2(\mathbf{R} \times [0,\infty))$ function and solves* (6.1).

Proof. The proof is a standard calculation using the First Fundamental Theorem of Calculus. □

6.2 Causality

D'Alembert's formula (6.3) shows us that the solution of the wave equation $u(x,t)$ at a point (x,t) is influenced only by the initial data within a certain range of values. More precisely, we can see that $u(x,t)$ depends only on the values of g at $x-ct$ and $x+ct$ and the values of h between $x-ct$ and $x+ct$. With this fact in mind, we call the region $D = \{(y,s) \in \mathbf{R}^2_+ \,|\, x - c(t-s) \le y \le x + c(t-s)\}$ the *domain of dependence* of the point (x,t) (see Figure 6(a)).

Turning the argument on its head, the values of the data at $(x,0)$ only affect the solution at points (y,s) such that $|y-x| \le cs$ so $I = \{(y,s) \in \mathbf{R}^2_+ \,|\, x - ct \le y \le x + ct\}$ is called the *domain of influence* of the point $(x,0)$ (see Figure 6(b)).

But why are we talking about regions in $\mathbf{R}^2_+$ when the data is given on the boundary $\partial\mathbf{R}^2_+$ of the upper-half plane? This is because we can generalise d'Alembert's formula to a wave equation with a source term:

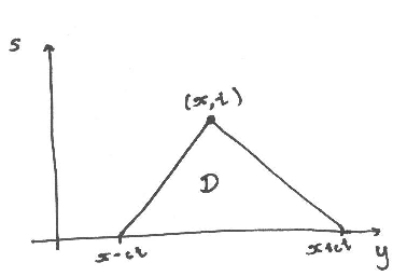
$$\begin{cases} \partial_t^2 u(x,t) - c^2\partial_x^2 u(x,t) = f(x,t) & \text{for } x \in \mathbf{R} \text{ and } t > 0, \\ u(x,0) = g(x) \quad \text{and} \quad \partial_t u(x,0) = h(x) & \text{for } x \in \mathbf{R}. \end{cases} \tag{6.4}$$

The function $f\colon \overline{\mathbf{R}^2_+} \to \mathbf{R}$ is called a source as physically it can represent an external applied force, which is a source of energy for the physical system. (We will discuss energy further in Section 6.3.) The following theorem, which identifies a solution to (6.4), also shows us that the solution u at a point (x,t) only depends on the values of f in the domain of dependence of the point (x,t).

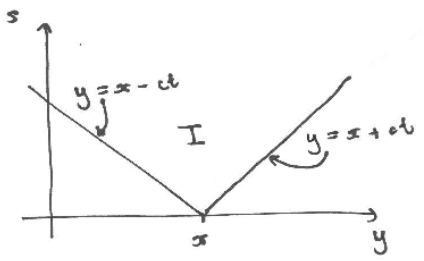
Theorem 6.2. *Assume that $g \in C^2(\mathbf{R})$, $h \in C^1(\mathbf{R})$ and $f \in C^1(\overline{\mathbf{R}^2_+})$. Then u defined by*

$$u(x,t) = \frac{1}{2}\left(g(x+ct) + g(x-ct)\right) + \frac{1}{2c}\int_{x-ct}^{x+ct} h(y)dy + \frac{1}{2c}\int_0^t \int_{x-c(t-s)}^{x+c(t-s)} f(y,s)dyds \tag{6.5}$$

is a $C^2(\mathbf{R} \times [0,\infty))$ function and solves (6.4).



(a) The domain of dependence D of a point (x,t) is the region enclosed by the triangle with vertices (x,t), $(x-ct,0)$ and $(x+ct,0)$.



(b) The domain of influence I of a point $(x,0)$ is the wedge with vertex at $(x,0)$ and two edges with equations $y = x-ct$ and $y = x+ct$.

Figure 6: Causality for the wave equation

Proof. We recognise the first two terms in (6.5) from (6.3), so we know these two terms provide a solution to (6.1). Since the wave equation is linear, it only remains to check that the last term in (6.5)

$$v(x,t) = \frac{1}{2c}\int_0^t \int_{x-c(t-s)}^{x+c(t-s)} f(y,s)dyds$$

is a $C^2(\mathbf{R}\times[0,\infty))$ function and solves

$$\begin{cases} \partial_t^2 v(x,t) - c^2\partial_x^2 v(x,t) = f(x,t) & \text{for } x\in\mathbf{R} \text{ and } t>0, \\ v(x,0) = 0 \quad \text{and} \quad \partial_t v(x,0) = 0 & \text{for } x\in\mathbf{R}. \end{cases}$$

Clearly $v(x,0)=0$. We also have

$$\begin{aligned} \partial_t v(x,t) &= \frac{1}{2c}\int_x^x f(y,t)dy + \frac{1}{2c}\int_0^t cf(x+c(t-s),s) + cf(x-c(t-s),s)ds \\ &= \frac{1}{2}\int_0^t f(x+c(t-s),s) + f(x-c(t-s),s)ds, \end{aligned}$$

so, in particular, $\partial_t v(x,0)=0$. Furthermore

$$\begin{aligned} \partial_{tt} v(x,t) &= \frac{1}{2}(f(x,t)+f(x,t)) + \frac{c}{2}\int_0^t \partial_1 f(x+c(t-s),s) - \partial_1 f(x-c(t-s),s)ds \\ &= f(x,t) + \frac{c}{2}\int_0^t \partial_1 f(x+c(t-s),s) - \partial_1 f(x-c(t-s),s)ds \end{aligned}$$

and

$$\partial_x v(x,t) = \frac{1}{2c}\int_0^t f(x+c(t-s),s) - f(x-c(t-s),s)ds,$$

so

$$\partial_{xx} v(x,t) = \frac{1}{2c}\int_0^t \partial_1 f(x+c(t-s),s) - \partial_1 f(x-c(t-s),s)ds.$$

Therefore

$$\begin{aligned} \partial_{tt} v(x,t) - c^2\partial_{xx} v(x,t) &= f(x,t) + \frac{c}{2}\int_0^t \partial_1 f(x+c(t-s),s) - \partial_1 f(x-c(t-s),s)ds \\ &\quad - \frac{c}{2}\int_0^t \partial_1 f(x+c(t-s),s) - \partial_1 f(x-c(t-s),s)ds \\ &= f(x,t). \end{aligned}$$

Finally, we see that both $\partial_{tt}v$ and $\partial_{xx}v$ are continuous and we can also compute

$$\partial_{tx}v(x,t) = \partial_{xt}v(x,t) = \frac{1}{2}\int_0^t \partial_1 f(x+c(t-s),s) + \partial_1 f(x-c(t-s),s)ds,$$

which is continuous too, so $v \in C^2(\mathbf{R}\times[0,\infty))$. □

6.3 Energy

Recall from (3.1) that $c^2 = T/\rho$ where T is tension and ρ is mass density. Adjusting our point of view from the two dimensional motivation ($n = 2$) in Section 3.1 to that of one spatial dimension ($n = 1$) a reasonable physical situation to have in mind is that of a vibrating string. The mass density ρ is now mass per unit length of string and the tension T is the force acting tangent to the string. A solution $u(x,t)$ to the wave equation represents the vertical displacement the string at a given horizontal coordinate x and time t. We know from physics that the energy associated with motion (kinetic energy) is given by half of the mass times velocity squared. Thus the kinetic energy per unit length at position x and time t is given by $\frac{1}{2}\rho(\partial_t u(x,t))^2$, and so the kinetic energy of the whole string is

$$\frac{1}{2}\int_{-\infty}^{\infty}\rho(\partial_t u(x,t))^2 dx.$$

The elastic energy stored in the string by virtue of its shape (potential energy) is given by the deformation times the force exerted while performing that deformation. The force acting as the string stretches and contracts will be T and thus constant. The length of the string at a given time t is given by the length of the graph of $x \mapsto u(x,t)$, which is

$$\int_{-\infty}^{\infty}\sqrt{1+(\partial_x u(x,t))^2}dx.$$

Thus the change in the length of the string, compared to when it is not deformed at all ($u(x,t) = 0$) is

$$\int_{-\infty}^{\infty}\left(\sqrt{1+(\partial_x u(x,t))^2}-1\right)dx \approx \frac{1}{2}\int_{-\infty}^{\infty}(\partial_x u(x,t))^2 dx,$$

and so we take the potential energy to be

$$\frac{1}{2}\int_{-\infty}^{\infty}T(\partial_x u(x,t))^2 dx.$$

We define the *energy* of u at time t to be the sum of the kinetic and potential energy:

$$E[u](t) := \frac{1}{2}\int_{-\infty}^{\infty}\rho(\partial_t u(x,t))^2 + T(\partial_x u(x,t))^2 dx. \tag{6.6}$$

Although energy will be transformed from kinetic to potential and back again as the string vibrates, we would expect the total energy to be conserved. This is the content of the next theorem.

Theorem 6.3. *Assume that $u \in C^2(\mathbf{R}\times[0,\infty))$ solves $\partial_{tt}u(x,t) - c^2\partial_{xx}u(x,t) = 0$ (with $c^2 = T/\rho$), is such that $\partial_t u(x,t) \to 0$ and $\partial_x u(x,t) \to 0$ as $x \to \pm\infty$, and the integrals*

$$\int_{-\infty}^{\infty}|\partial^\alpha u(x,t)|^2 dx$$

converge uniformly in t, where ∂^α is any derivative of order less than or equal to two.[6] *Then $E[u]$ defined in* (6.6) *is a constant function.*

[6] For those who are familiar with the notation, α is a multi-index with order $|\alpha| \le 2$.

Proof. Differentiating the kinetic energy and using the wave equation u solves, we have

$$\begin{aligned}\frac{d}{dt}\left(\frac{1}{2}\int_{-\infty}^{\infty}\rho(\partial_t u(x,t))^2dx\right) &= \frac{1}{2}\int_{-\infty}^{\infty}\rho\partial_t u(x,t)\partial_{tt}u(x,t)dx \\ &= \frac{1}{2}\int_{-\infty}^{\infty}T\partial_t u(x,t)\partial_{xx}u(x,t)dx = -\frac{1}{2}\int_{-\infty}^{\infty}T\partial_{tx}u(x,t)\partial_x u(x,t)dx \\ &= -\frac{d}{dt}\left(\frac{1}{2}\int_{-\infty}^{\infty}T(\partial_x u(x,t))^2dx\right).\end{aligned}$$

Therefore

$$\frac{d}{dt}\left(\frac{1}{2}\int_{-\infty}^{\infty}\rho(\partial_t u(x,t))^2 + T(\partial_x u(x,t))^2dx\right) = 0$$

and the theorem is proved. □

Remark 6.4. *We can modify the defintion of energy by a multiplicative factor and we would still have a conserved quantity. Indeed if we modified the definition by dividing by ρ, the energy would be*

$$\frac{1}{2}\int_{-\infty}^{\infty}(\partial_t u(x,t))^2 + c^2(\partial_x u(x,t))^2dx$$

which is an expression which only involves constants (namely c) which directly appear in the wave equation. However, the definition we have taken is consistent with that used in physics.

Corollary 6.5. *(a) For any given functions g and h, there is at most one solution u to* (6.1) *which satisfies the same hypothesis as in Theorem 6.3.*

(b) For any given functions g, h and f, there is at most one solution u to (6.4) *which satisfies the same hypothesis as in Theorem 6.3.*

Proof. In both cases the difference of two solutions $w = u_1 - u_2$ solves (6.1) with $g = h = 0$. Therefore, by Theorem 6.3,

$$\frac{1}{2}\int_{-\infty}^{\infty}\rho(\partial_t w(x,t))^2 + T(\partial_x w(x,t))^2dx = E[w](t) = E[w](0) = 0.$$

In particular this implies $\partial_t w(x,t) = 0$, so $w(x,t)$ is a function of x only and in particular $w(x,t) = w(x,0)$. But this function must be zero, since $w(x,0) = 0$. □

6.4 Reflections

6.4.1 Waves on the half-line

So far we have only considered the wave equation on the real line, which would model the motion of a vibrating string which is infinitely long. This is perhaps slightly unrealistic, as we are much more likely to encounter strings of finite length in the real world. In this section we will consider a situation which could be described as half-way between an infinitely long string and a finite length string. In Section 6.4.2 we will extend the method used here to deal with the finite case.

We will consider the wave equation on the positive half-line with a Dirichlet boundary condition. Given $g, h\colon [0,\infty) \to \mathbf{R}$ we wish to find $v\colon [0,\infty)\times[0,\infty) \to \mathbf{R}$ such that

$$\begin{cases} \partial_{tt}v(x,t) - c^2\partial_{xx}v(x,t) = 0 & \text{for } x \in (0,\infty) \text{ and } t > 0, \\ v(x,0) = g(x) \quad \text{and} \quad \partial_t v(x,0) = h(x) & \text{for } x \in [0,\infty), \text{ and} \\ v(0,t) = 0 & \text{for } t > 0. \end{cases} \tag{6.7}$$

We can relate (6.7) to the analogous problem (6.1) on the whole real line. Suppose u solved (6.1) with initial values g_{odd} and h_{odd}, the odd extensions of g and h:

$$g_{\text{odd}}(x) := \begin{cases} g(x) & \text{if } x \geq 0, \text{ and} \\ -g(-x) & \text{if } x < 0; \end{cases}$$

and

$$h_{\text{odd}}(x) := \begin{cases} h(x) & \text{if } x \geq 0, \text{ and} \\ -h(-x) & \text{if } x < 0. \end{cases}$$

Homework exercise 7.2 shows that

$$v(x,t) = \frac{1}{2}\left(g_{\text{odd}}(x+ct) + g_{\text{odd}}(x-ct)\right) + \frac{1}{2c}\int_{x-ct}^{x+ct} h_{\text{odd}}(y)dy \tag{6.8}$$

would be an odd function for each $t > 0$. Thus, in particular $v(0,t) = 0$ for all $t > 0$, and $v(x,0) = g(x)$ and $\partial_t v(x,0) = h(x)$ for all $x \in [0,\infty)$, so u restricted to $x \geq 0$ is the solution to (6.7) we are looking for.

Observe that if (6.8) is to be a solution to (6.1) then according to Theorem 6.1 we need to know that $g_{\text{odd}} \in C^2(\mathbf{R})$ and $h_{\text{odd}} \in C^1(\mathbf{R})$. This will only be the case if $g \in C^2([0,\infty))$ and $h \in C^1([0,\infty))$ and $g(0) = h(0) = 0$.

We formulate the preceeding discussion as a theorem.

Theorem 6.6. *Suppose $g \in C^2([0,\infty))$, $h \in C^1([0,\infty))$ and $g(0) = h(0) = 0$. Then the function $v\colon [0,\infty)\times[0,\infty) \to \mathbf{R}$ defined by*

$$v(x,t) = \frac{1}{2}\left(g_{odd}(x+ct) + g_{odd}(x-ct)\right) + \frac{1}{2c}\int_{x-ct}^{x+ct} h_{odd}(y)dy.$$

for $x \geq 0$ and $t \geq 0$ is a $C^2([0,\infty)\times[0,\infty))$ function which solves (6.7).

6.4.2 Waves on a finite interval

Now consider the wave equation on a finite interval $[0,\ell]$ with Dirichlet boundary conditions. Given $g, h\colon [0,\ell] \to \mathbf{R}$ we wish to find $v\colon [0,\ell]\times[0,\infty) \to \mathbf{R}$ such that

$$\begin{cases} \partial_{tt}v(x,t) - c^2\partial_{xx}v(x,t) = 0 & \text{for } x \in (0,\ell) \text{ and } t > 0, \\ v(x,0) = g(x) \quad \text{and} \quad \partial_t v(x,0) = h(x) & \text{for } x \in [0,\ell], \text{ and} \\ v(0,t) = 0 \quad \text{and} \quad v(\ell,t) = 0 & \text{for } t > 0. \end{cases} \tag{6.9}$$

Once again, we can relate (6.9) to the analogous problem (6.1) on the whole real line. Suppose u solved (6.1) with initial values g_{ext} and h_{ext}, the following extensions of g and h:

$$g_{\text{ext}}(x) := \begin{cases} g(x - 2\ell n) & \text{if } x \in [2\ell n, 2\ell n + \ell] \text{ for some } n \in \mathbf{Z}, \\ -g(-x + 2\ell n) & \text{if } x \in (2\ell n - \ell, 2\ell n) \text{ for some } n \in \mathbf{Z}; \end{cases}$$

so g_{ext} is an odd extension of g with respect to both $x = 0$ and $x = \ell$ (and also 2ℓ-periodic), and

$$h_{\text{ext}}(x) := \begin{cases} h(x - 2\ell n) & \text{if } x \in [2\ell n, 2\ell n + \ell] \text{ for some } n \in \mathbf{Z}, \\ -h(-x + 2\ell n) & \text{if } x \in (2\ell n - \ell, 2\ell n) \text{ for some } n \in \mathbf{Z}; \end{cases}$$

so h_{ext} is also an odd extension of h with respect to both $x = 0$ and $x = \ell$ (and 2ℓ-periodic).

Homework exercise 7.2 and the translation invariance of the wave equation proved in exercise 7.5a shows that

$$u(x,t) = \frac{1}{2}\left(g_{\text{ext}}(x+ct) + g_{\text{ext}}(x-ct)\right) + \frac{1}{2c}\int_{x-ct}^{x+ct} h_{\text{ext}}(y)dy$$

would be an odd function with respect to both $x = 0$ and $x = \ell$ for each $t > 0$. Thus, in particular $u(0,t) = 0$ and $u(\ell,t) = 0$ for all $t > 0$, and $v(x,0) = g(x)$ and $\partial_t v(x,0) = h(x)$ for all $x \in [0,\ell]$, so u restricted to $0 \leq x \leq \ell$ is the solution to (6.9) we are looking for.

We must also once again impose conditions on g and h that ensure g_{ext} and h_{ext} are suitable smooth. All these considerations give us the following theorem.

Theorem 6.7. *Suppose $g \in C^2([0,\ell])$, $h \in C^1([0,\ell])$ and $g(0) = h(0) = g(\ell) = h(\ell) = 0$. Then the function $v\colon [0,\infty)\times[0,\infty) \to \mathbf{R}$ defined by*

$$v(x,t) = \frac{1}{2}\left(g_{ext}(x+ct) + g_{ext}(x-ct)\right) + \frac{1}{2c}\int_{x-ct}^{x+ct} h_{ext}(y)dy.$$

for $0 \leq x \leq \ell$ and $t \geq 0$ is a $C^2([0,\ell]\times[0,\infty))$ function which solves (6.9).

6.5 Higher dimensions

6.5.1 Three spatial dimensions: spherical means

In this section we will derive a formula for solutions $u\colon \mathbf{R}^3 \times [0,\infty) \to \mathbf{R}$ to the wave equation

$$\partial_{tt}u(x,y,z,t) - (\partial_{xx} + \partial_{yy} + \partial_{zz})u(x,y,z,t) = 0 \quad \text{for } t > 0 \text{ and } (x,y,z) = \mathbf{x} \in \mathbf{R}^3 \tag{6.10}$$

(where for simplicity we set $c = 1$) with the initial conditions

$$u(\mathbf{x},0) = \phi(\mathbf{x}), \quad \text{and} \quad \partial_t u(\mathbf{x},0) = \psi(\mathbf{x}) \quad \text{for } \mathbf{x} \in \mathbf{R}^3.$$

This will be achieved by studying the properties of *spherical means* $\overline{u}_{\mathbf{x}}$ of u about a fixed $\mathbf{x} \in \mathbf{R}^3$ defined to be

$$\overline{u}_{\mathbf{x}}(r,t) = \frac{1}{4\pi r^2}\int_{|\mathbf{y}-\mathbf{x}|=r} u(\mathbf{y},t)d\sigma(\mathbf{y}) \quad \text{for } t, r > 0.$$

We begin by applying the Divergence Theorem to a solution u to (6.10) in the ball $B_r(\mathbf{x}) = \{\mathbf{y} \in \mathbf{R}^n \,|\, |\mathbf{y}-\mathbf{x}| < r\}$:

$$\int_{B_r(\mathbf{x})} \partial_{tt}u(\mathbf{y},t)d\mathbf{y} = \int_{B_r(\mathbf{x})} \Delta u(\mathbf{y},t)d\mathbf{y} = \int_{\partial B_r(\mathbf{x})} \mathbf{n}\cdot\nabla u(\mathbf{y},t)d\sigma(\mathbf{y}) \tag{6.11}$$

which can be rewritten in polar coordinates as

$$\int_0^r\int_0^{2\pi}\int_0^{\pi} (\partial_{tt}u)\rho^2\sin\theta d\theta d\phi d\rho = \int_0^{2\pi}\int_0^{\pi} (\partial_r u)r^2\sin\theta d\theta d\phi$$

and simplified to

$$\int_0^r \rho^2 \partial_{tt}\overline{u}_{\mathbf{x}}(\rho,t)d\rho = r^2\partial_r\overline{u}_{\mathbf{x}}(r,t).$$

Differentiating with respect to r gives

$$r^2\partial_{tt}\overline{u}_{\mathbf{x}}(r,t) = r^2\partial_{rr}\overline{u}_{\mathbf{x}}(r,t) + 2r\partial_r\overline{u}_{\mathbf{x}}(r,t). \tag{6.12}$$

With the substitution $v(r,t) = r\overline{u}_{\mathbf{x}}(r,t)$ we have $\partial_{tt}v(r,t) = r\partial_{tt}\overline{u}_{\mathbf{x}}(r,t)$ and $\partial_{rr}v(r,t) = r\partial_{rr}\overline{u}_{\mathbf{x}}(r,t) + 2\partial_r\overline{u}_{\mathbf{x}}(r,t)$ so that, dividing (6.12) by r, we obtain

$$\partial_{tt}v(r,t) = \partial_{rr}v(r,t) \quad \text{for } r,t > 0. \tag{6.13}$$

Moreover $v(0,t) = 0 \times u(0,t) = 0$, so v satisfies (6.7) for some g and h. We now wish to make use of (6.8), so we must calculate the initial values g and h appearing in (6.7). Clearly

$$v(r,0) = r\overline{\phi}_{\mathbf{x}}(r) \quad \text{and} \quad \partial_t v(r,0) = r\overline{\psi}_{\mathbf{x}}(r),$$

with

$$\overline{\phi}_{\mathbf{x}}(r) := \frac{1}{4\pi r^2}\int_{|\mathbf{y}-\mathbf{x}|=r}\phi(\mathbf{y})d\sigma(\mathbf{y}) \quad \text{and} \quad \overline{\psi}_{\mathbf{x}}(r) := \frac{1}{4\pi r^2}\int_{|\mathbf{y}-\mathbf{x}|=r}\psi(\mathbf{y})d\sigma(\mathbf{y}).$$

Therefore rewriting (6.8) for the present case gives that

$$v(r,t) = \frac{\partial}{\partial t}\left(\frac{1}{2}\int_{t-r}^{t+r} s\overline{\phi}_{\mathbf{x}}(s)ds\right) + \frac{1}{2}\int_{t-r}^{t+r} s\overline{\psi}_{\mathbf{x}}(s)ds$$

at least in the case $0 \le r \le t$ (see homework 8.4).

We can now recover $u(\mathbf{x},t)$ as

$$u(\mathbf{x},t) = \lim_{r\to 0}\overline{u}_{\mathbf{x}}(r,t) = \lim_{r\to 0}\frac{v(r,t)}{r} = \lim_{r\to 0}\frac{v(r,t)-v(0,t)}{r} = \partial_r v(0,t).$$

We calculate

$$\partial_r v(r,t) = \frac{\partial}{\partial t}\left(\frac{1}{2}\left((t+r)\overline{\phi}_{\mathbf{x}}(t+r) + (t-r)\overline{\phi}_{\mathbf{x}}(t-r)\right)\right) + \frac{1}{2}\left((t+r)\overline{\psi}_{\mathbf{x}}(t+r) + (t-r)\overline{\psi}_{\mathbf{x}}(t-r)\right)$$

so

$$u(\mathbf{x},t) = \frac{\partial}{\partial t}\left(t\overline{\phi}_{\mathbf{x}}(t)\right) + t\overline{\psi}_{\mathbf{x}}(t) = \frac{\partial}{\partial t}\left(\frac{1}{4\pi t}\int_{|\mathbf{y}-\mathbf{x}|=t}\phi(\mathbf{y})d\sigma(\mathbf{y})\right) + \frac{1}{4\pi t}\int_{|\mathbf{y}-\mathbf{x}|=t}\psi(\mathbf{y})d\sigma(\mathbf{y}). \tag{6.14}$$

Thus we have derived a formula for a solution to the wave equation (6.10) in three spatial dimensions by relating it to a similar problem for the wave equation (6.7) in one spatial dimension. This formula (6.14) is called *Kirchoff's formula*.

Observe that the solution $u(\mathbf{x},t)$ only depends on the initial data at values $\mathbf{y}$ lying in the sphere $|\mathbf{y}-\mathbf{x}| = t$. This is called *Huygen's Principle*. A consequence of this is that the sound transmitted by a speaker in three dimensional space sounds the same to a listener regardless of the distance between the speaker and listener. As we have seen, this is not the case in one dimensional space. Indeed, in one dimension d'Alemberts formula (6.3) (say with $c = 1$) shows that the solution depends not just on the the data a distance t from the listener, but all distances up to t. Thus sound transmitted by a speaker will sound different depending on the distance between the speaker and the listener. In Section 6.5.2 we will see this is also the case in two dimensions. In general Huygen's Principle holds in odd dimensions greater than one and does not hold in even dimensions.

6.5.2 Two spatial dimensions: the method of descent

With the help of Kirchoff's formula (6.14) in three spatial dimensions it is easy to derive a formula for the solution to the initial value problem

$$\begin{cases} \partial_{tt}v(x,y,t) - (\partial_{xx}+\partial_{yy})v(x,y,t) = 0 & \text{for } (x,y)\in\mathbf{R}^2 \text{ and } t>0, \\ v(x,y,0) = \phi(x,y) \quad \text{and} \quad \partial_t v(x,y,0) = \psi(x,y) & \text{for } (x,y)\in\mathbf{R}^2. \end{cases} \tag{6.15}$$

We do this by viewing a solution to (6.15) as a solution to (6.10) which happens to be constant in the z-direction. Kirchoff's formula (6.14) says

$$\begin{aligned} u(x,y,t) &= \frac{\partial}{\partial t}\left(\frac{1}{4\pi t}\int_{(x-a)^2+(y-b)^2+(z-c)^2=t^2}\phi(a,b)d\sigma(a,b,c)\right) \\ &\quad + \frac{1}{4\pi t}\int_{(x-a)^2+(y-b)^2+(z-c)^2=t^2}\psi(a,b)d\sigma(a,b,c) \\ &= \frac{\partial}{\partial t}\left(\frac{1}{4\pi t}\int_{a^2+b^2+c^2=t^2}\phi(a+x,b+y)d\sigma(a,b,c)\right) \\ &\quad + \frac{1}{4\pi t}\int_{a^2+b^2+c^2=t^2}\psi(a+x,b+y)d\sigma(a,b,c). \end{aligned}$$

We can parametrise the sphere $a^2+b^2+c^2 = t^2$ in the variables a and b with two hemispheres $c = \pm\sqrt{t^2-a^2-b^2}$, so that the domain of integration in a and b becomes the disc $\{(a,b)\,|\,a^2+b^2\le t^2\}$ We find that

$$d\sigma(a,b,c) = \sqrt{1+\left(\frac{\partial c}{\partial a}\right)^2+\left(\frac{\partial c}{\partial b}\right)^2}dadb = \sqrt{\frac{((t^2-a^2-b^2)+a^2+b^2)\,dadb}{t^2-a^2-b^2}} = \frac{tdadb}{\sqrt{t^2-a^2-b^2}}$$

so

$$\begin{aligned} u(x,y,t) &= \frac{\partial}{\partial t}\left(\frac{1}{2\pi}\int_{a^2+b^2\le t^2}\frac{\phi(a+x,b+y)}{\sqrt{t^2-a^2-b^2}}dadb\right) \\ &\quad + \frac{1}{2\pi}\int_{a^2+b^2\le t^2}\frac{\psi(a+x,b+y)}{\sqrt{t^2-a^2-b^2}}dadb. \end{aligned} \tag{6.16}$$

This formula proves the claim we made in Section 6.5.1 that Huygen's Principle does not hold in two dimensions. The solution $u(x, y, t)$ from (6.16) depends on the data in a disc of radius t about (x, y), not just on the circle of radius t centred at (x, y).[7]

7 The heat equation

We now move on to study another PDE that appeared in Section 3, namely the heat equation (Section 3.2). For simplicity we will take the proportionality constant k that appeared there to be equal to one. We will pose similar questions to those we asked regarding Laplace's equation and the wave equation, but we will see that the answers demonstrate there are differences between the PDEs as well as similarities.

7.1 Another maximum principle

In this section we will consider solutions $u\colon \overline{\Omega}\times[0,T] \to \mathbf{R}$ to the heat equation $\partial_t u(\mathbf{x},t) - \Delta u(\mathbf{x},t) = 0$, where $\Omega \subset \mathbf{R}^n$ is an open bounded connected set and $T > 0$. We begin with a property that is very similar to one exhibited by harmonic functions. It's proof is also similar to the case of harmonic functions, but we repeat it in detail here for completeness.

Theorem 7.1 (Weak Maximum Principle)**.** *Suppose $\Omega \subset \mathbf{R}^n$ is an open bounded connected set and $T > 0$. Let $u\colon \overline{\Omega} \times [0,T] \to \mathbf{R}$ be a continuous function which is also a solution to the heat equation $\partial_t u(\mathbf{x},t) - \Delta u(\mathbf{x},t) = 0$ for $(\mathbf{x},t) \in \Omega \times (0,T]$. Then the maximum value of u is attained at a point $(\mathbf{x},t) \in \overline{\Omega} \times [0,T]$ such that either $t = 0$ or $\mathbf{x} \in \partial\Omega$.*

Remark 7.2. *Theorem 7.1 says that the maximum of u is either obtained initially ($t = 0$) or on the lateral edges of the domain ($\mathbf{x} \in \partial\Omega$).*

Theorem 7.1 does not rule out the possibility that the maximum is also obtained in $\Omega \times (0,T]$. It turns out, however, that one can rule out such a possibility, although the proof is much more difficult, so we will not do this here.

Just as for Theorem 5.1, we can make an analogous statement about the minimum of u.

Proof of Theorem 7.1. For $\varepsilon > 0$ set $v(\mathbf{x},t) = u(\mathbf{x},t) + \varepsilon|\mathbf{x}|^2$. Since v is continuous on the compact set $\overline{\Omega} \times [0,T]$ it must attain a maximum somewhere in $\overline{\Omega} \times [0,T]$.

Suppose v attains this maximum at $(\mathbf{x},t)$ with $\mathbf{x} \in \Omega$ and $0 < t \leq T$, then, by the first derivative test, $\partial_t u(\mathbf{x},t) = 0$ and by the second derivative test, $\Delta v(\mathbf{x}) = \sum_{j=1}^n \partial_j^2 v(\mathbf{x}) \leq 0$. This means

$$\partial_t v(\mathbf{x},t) - \Delta v(\mathbf{x},t) \geq 0 - 0 = 0.$$

On the other hand, since u solves the heat equation, we can compute

$$\partial_t v(\mathbf{x},t) - \Delta v(\mathbf{x},t) = \partial_t u(\mathbf{x},t) - \Delta u(\mathbf{x},t) - 2n\varepsilon = 0 - 2n\varepsilon < 0,$$

which is a contradiction.

Therefore v must attain its maximum at a point $(\mathbf{x},t)$ for which either $\mathbf{x} \in \partial\Omega$ or $t = 0$. Set $M = \max_{(\mathbf{x},t)\in B} u(\mathbf{x},t)$ where $B = (\Omega \times \{0\}) \cup (\partial\Omega \times (0,T])$, then

$$\max_{\overline{\Omega}\times[0,T]} u \leq \max_{\overline{\Omega}\times[0,T]} v \leq \max_B v \leq \max_B u + \varepsilon D = M + \varepsilon D.$$

Since ε is arbitrary we must have $\max_{\overline{\Omega}\times[0,T]} u \leq M$. □

Theorem 7.1 can be used to prove the uniqueness of solutions to initial boundary value problems for the heat equation (see homework exercise 9.2(b)), however we will use the energy method below to prove the same result.

[7] A circle and a disc are the two dimensional versions of a sphere and a ball, respectively.

7.2 Uniqueness and stability via the energy method

Consider the initial boundary value problem

$$\begin{cases} \partial_t u(\mathbf{x},t) - \Delta u(\mathbf{x},t) = 0 & \text{for } \mathbf{x} \in \Omega \text{ and } t \in (0,T]; \\ u(\mathbf{x},0) = \phi(x) & \text{for } \mathbf{x} \in \overline{\Omega}; \text{ and} \\ u(\mathbf{y},t) = g(\mathbf{y},t) & \text{for } \mathbf{y} \in \partial\Omega \text{ and } t \in (0,T]. \end{cases} \tag{7.1}$$

One can show that if $g = 0$, the quantity

$$\int_\Omega |u(\mathbf{x},t)|^2 d\mathbf{x}$$

is a decreasing function of t. Indeed, suppose $u \in C^1(\overline{\Omega} \times [0,T])$ and is also a solution to (7.1). Then using (5.8)

$$\begin{aligned} &\frac{d}{dt}\int_\Omega |u(\mathbf{x},t)|^2 d\mathbf{x} = \int_\Omega u(\mathbf{x},t)\partial_t u(\mathbf{x},t) d\mathbf{x} \\ &= \int_\Omega u(\mathbf{x},t)\Delta u(\mathbf{x},t) d\mathbf{x} = -\int_\Omega \nabla u(\mathbf{x},t)\nabla u(\mathbf{x},t) d\mathbf{x} = -\int_\Omega |\nabla u(\mathbf{x},t)|^2 d\mathbf{x} \le 0. \end{aligned}$$

In particular, we have

$$0 \le \int_{\mathbf{R}^n} |u(\mathbf{x},t)|^2 d\mathbf{x} \le \int_{\mathbf{R}^n} |\phi(\mathbf{x})|^2 d\mathbf{x}$$

for all $t \in [0,T]$. This means that if we had two solutions u_1 and u_2 of (7.1), then their difference $w = u_2 - u_2$ would satsify (7.1) with $\phi = 0$ and $g = 0$, so

$$0 \le \int_{\mathbf{R}^n} |u_2(\mathbf{x},t) - u_1(\mathbf{x},t)|^2 d\mathbf{x} = \int_{\mathbf{R}^n} |w(\mathbf{x},t)|^2 d\mathbf{x} \le 0.$$

Whence $u_1 = u_2$. This proves the following theorm.

Theorem 7.3. *There is at most one function $u \in C^1(\overline{\Omega} \times [0,T])$ which is also a solution to* (7.1).

The same method also tells us the solution depends continuously on the data. Recall this was the third criteria, which we called stability, required in Section 4.4 for a problem to be well-posed.

Theorem 7.4. *Suppose $u_i \in C^1(\overline{\Omega} \times [0,T])$ solves* (7.1) *with $g = g_i$ and $\phi = \phi_i$ for $i = 1, 2$. If $g_1 = g_2$, then*

$$0 \le \int_\Omega |u_2(\mathbf{x},t) - u_1(\mathbf{x},t)|^2 d\mathbf{x} \le \int_\Omega |\phi_2(\mathbf{x}) - \phi_1(\mathbf{x})|^2 d\mathbf{x}$$

A similar, but different, stability (homework exercise 9.2(c)) can be proved for the heat equation using the Weak Maximum Principle (Theorem 7.1).

7.3 The initial value problem on the real line

Now consider the initial value problem

$$\begin{cases} \partial_t u(x,t) - \partial_{xx} u(x,t) = 0 & \text{for } x \in \mathbf{R} \text{ and } t \in (0,\infty); \\ u(x,0) = \phi(x) & \text{for } x \in \mathbf{R}. \end{cases} \tag{7.2}$$

In this section we will show that it is possible to find a solution to such a problem. To do this the function $S\colon \mathbf{R} \times (0,\infty) \to \mathbf{R}$ defined by

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

will be extremely important to us. This function is called the *heat kernel*. In Chapter 2.4 of Strauss a justification for studying this particular function is given, see also homework exercise 9.5.

Observe that

$$\partial_t S(x,t) = \frac{-1}{4\sqrt{\pi}t^{3/2}} e^{-x^2/4t} + \frac{x^2}{8\sqrt{\pi}t^{5/2}} e^{-x^2/4t}$$

and

$$\partial_x S(x,t) = -\frac{x}{4\sqrt{\pi}t^{3/2}} e^{-x^2/4t}$$

so

$$\partial_{xx} S(x,t) = -\frac{1}{4\sqrt{\pi}t^{3/2}} e^{-x^2/4t} + \frac{x^2}{8\sqrt{\pi}t^{5/2}} e^{-x^2/4t}.$$

This implies $\partial_t S(x,t) - \partial_{xx} S(x,t) = 0$, that is, S solves the heat equation.

For each $t > 0$ the function $x \mapsto S(x,t)$ is a Gaussian. You may have encountered such a function before in perhaps Calculus (as a function we can integrate on the real line without calculating a primative function) or probability theory (normal distributions). Observe that for small t the graph of $x \mapsto S(x,t)$ has a tall thin spike around zero and decays rapidly to zero as $|x|$ increases. For large t, the graph of $x \mapsto S(x,t)$ is fattened out, so that the spike at zero is more like a gentle hill. Consider the integral

$$u(x,t) = \int_{-\infty}^{\infty} S(x-y,t)\phi(y)dy. \tag{7.3}$$

If t is small, the integral in (7.3) would average ϕ over a very small interval near x. If we let $t \to 0$ we might expect these averages of ϕ near x to converge to $\phi(x)$. Moreover, because S solves the heat equation and the heat equation is translation invariant (that is, $(x,t) \mapsto S(x-y,t)$ is also a solution for each $y \in \mathbf{R}$) we expect (7.3) to also be a solution to the heat equation, as it is essentially a linear combination of solutions. This means, that we would guess that (7.3) would be a solution to (7.2). This guess is in fact correct, as the following proof shows.

Theorem 7.5. *Let $\phi\colon \mathbf{R} \to \mathbf{R}$ be a bounded continuous function. Then (7.3) defines an infinitely differentiable function on the set $\mathbf{R}^2_+ := \{(x,t) \mid x \in R, t > 0\}$, which satisfies $\partial_t u(x,t) - \partial_{xx} u(x,t) = 0$ for $(x,t) \in \mathbf{R}^2_+$ and $\lim_{t\to 0^+} u(x,t) = \phi(x)$ for each $x \in \mathbf{R}$.*

Proof. First we perform a change of variables

$$u(x,t) = \int_{-\infty}^{\infty} S(x-y,t)\phi(y)dy = \int_{-\infty}^{\infty} S(z,t)\phi(x-z)dz = \int_{-\infty}^{\infty} S(p\sqrt{t},t)\phi(x-p\sqrt{t})\sqrt{t}dp.$$

Then it is easy to see that $S(p\sqrt{t},t)\phi(p\sqrt{t}-x)\sqrt{t} = \frac{e^{-p^2/4}}{2\sqrt{\pi}}\phi(p\sqrt{t}-x)$. This means that the integrand is bounded above by $\frac{1}{2\sqrt{\pi}} \sup_{y\in\mathbf{R}} |\phi(y)| e^{-p^2/4}$, so the integral in p above converges uniformly in x and t.

Moreover, $u(x,t)$ will be differentiable any number of times with respect to x or t, say α times, where α is a multi-index, and equal to

$$\partial^\alpha u(x,t) = \int_{-\infty}^{\infty} \partial^\alpha S(x-y,t)\phi(y)dy$$

provided we can justify interchanging differentiation and integration. To justify this is suffices to show the integrand above is uniformly integrable. This can be done just as before, since differentiating S just introduces a polynomial in p in front of $e^{-p^2/4}$ (together with factors of t). This polynomial growth is not enough to destroy the uniform convergence of the integral due to the exponential decay $e^{-p^2/4}$. For example,

$$\int_{-\infty}^{\infty} \partial_1 S(x-y,t)\phi(y)dy = \int_{-\infty}^{\infty} \partial_1 S(z,t)\phi(z-x)dz = \int_{-\infty}^{\infty} \partial_1 S(p\sqrt{t},t)\phi(p\sqrt{t}-x)\sqrt{t}dp.$$

Since $\partial_1 S(x,t) = -\frac{x}{4\sqrt{\pi}t^{3/2}} e^{-x^2/4t}$, we have that $\partial_1 S(p\sqrt{t},t)\phi(p\sqrt{t}-x)\sqrt{t} = -\frac{pe^{-p^2/4}}{4\sqrt{\pi t}}\phi(p\sqrt{t}-x)$ so, because $|\partial_1 S(p\sqrt{t},t)\phi(p\sqrt{t}-x)\sqrt{t}| \le \frac{pe^{-p^2/4}}{4\sqrt{\pi t}} \sup_{y\in\mathbf{R}} |\phi(y)|$, we see that $\partial_1 S(p\sqrt{t},t)\phi(p\sqrt{t}-x)\sqrt{t}$ is integrable in p uniformly in $x \in \mathbf{R}$ and $t > \delta$ for each fixed $\delta > 0$.

Now we know that we can justify interchanging differentiation and integration, it follows from the fact that S solves the heat equation, that (7.3) also solves the heat equation.

It remains to prove the initial condition holds. We can calculate that

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

Therefore

$$\begin{aligned} u(x,t) - \phi(x) &= \int_{-\infty}^{\infty} S(x-y,t)(\phi(y)-\phi(x))dy = \int_{-\infty}^{\infty} S(p\sqrt{t},t)(\phi(p\sqrt{t}-x)-\phi(x))\sqrt{t}dp \\ &= \int_{-\infty}^{\infty} \frac{1}{2\sqrt{\pi}} e^{-p^2/4}(\phi(p\sqrt{t}-x)-\phi(x))dp. \end{aligned}$$

The idea of the proof from here is to split the integral in two. The integral over p close to the origin will be small because $|\phi(p\sqrt{t}-x)-\phi(x)|$ will be small if t is small. Recalling that the graph of $p \mapsto \frac{1}{2\sqrt{\pi}} e^{-p^2/4}$ will look like a bump centred at the origin and decay quickly away from the origin, the integral over large p will be also be small.

Fix $\varepsilon > 0$. We choose $\delta > 0$ so small that

$$\max_{|y-x|\leq\delta} |\phi(y) - \phi(x)| < \varepsilon/2$$

Then we rewrite the integral as

$$\begin{aligned} &\int_{-\infty}^{\infty} \frac{1}{2\sqrt{\pi}} e^{-p^2/4}(\phi(p\sqrt{t}-x)-\phi(x))dp \\ &= \int_{|p|<\delta/\sqrt{t}} \frac{1}{2\sqrt{\pi}} e^{-p^2/4}(\phi(p\sqrt{t}-x)-\phi(x))dp + \int_{|p|\geq\delta/\sqrt{t}} \frac{1}{2\sqrt{\pi}} e^{-p^2/4}(\phi(p\sqrt{t}-x)-\phi(x))dp \end{aligned}$$

We can bound the first integral using our choice of δ:

$$\left| \int_{|p|<\delta/\sqrt{t}} \frac{1}{2\sqrt{\pi}} e^{-p^2/4}(\phi(p\sqrt{t}-x)-\phi(x))dp \right| \leq \frac{\varepsilon}{2} \int_{|p|<\delta/\sqrt{t}} \frac{1}{2\sqrt{\pi}} e^{-p^2/4}dp \leq \frac{\varepsilon}{2},$$

since $\int_{|p|<\delta/\sqrt{t}} \frac{1}{2\sqrt{\pi}} e^{-p^2/4}dp \leq \int_{-\infty}^{\infty} \frac{1}{2\sqrt{\pi}} e^{-p^2/4}dp = 1$. The first integral can also be bounded using the boundedness of ϕ. If we take C to be the constant such that $|\phi(x)| \leq C$ for all $x \in \mathbf{R}$ (which exists since ϕ is bounded), then

$$\left| \int_{|p|\geq\delta/\sqrt{t}} \frac{1}{2\sqrt{\pi}} e^{-p^2/4}(\phi(p\sqrt{t}-x)-\phi(x))dp \right| \leq 2C \int_{|p|\geq\delta/\sqrt{t}} \frac{1}{2\sqrt{\pi}} e^{-p^2/4}dp.$$

We can make the last integral less than $\varepsilon/2$ since the last integral is just the 'tails' of a convergent integral, so will small for sufficiently small t. Thus we have proved $u(x,t) \to \phi(x)$ as $t \to 0$. □

7.4 A comparison of the wave and heat equations in one spatial dimension

We saw in Section 6.2 that the wave equation transmitted information at speed at most c.[8] The data that affected the solution at a given point (x,t) depended only on the data within the domain of dependence of (x,t). This made sense given the physical motivation for studying the equation.

At first sight it would be reasonable to expect the same of the heat equation. Heat can surely only flow from one place to another at a finite speed. However, a closer look at formula (7.3) shows this is not the case.

[8]Section 6.2 describes the result in one spatial dimension, but this can also be seen to hold in two and three spatial dimensions via formulae (6.14) and (6.16) respectively. Recall that we assumed $c = 1$ in those formulae, but a change of variables easily gives the result for arbitrary c.

Consider (7.2) with data ϕ given by

$$\phi(x) = \begin{cases} 1 - |x| & \text{for } |x| < 1; \\ 0 & \text{for } |x| \geq 1. \end{cases}$$

Formula (7.3) gives a solution to (7.2). Since S is positive it is clear that the solution $u(x,t)$ will also be positive for all $x \in \mathbf{R}$ and $t > 0$. Physically this says that the initial heat, which was localised to $|x| < 1$, has travelled an arbitrarily large distance in an arbitrarily small time. Consequently we do not have the finite speed of propagation we saw for the wave equation in the heat equation.

Theorem 7.5 shows that with just bounded and continuous data ϕ the solution to the heat equation (7.2) will be infinitely differentiable for $t > 0$. This is clearly not the case for the wave equation, as we can see from d'Alemberts formula (6.3). Thus it is reasonable to say that the heat equation is smoothing, but the wave equation is not.

In Table 1 we compare the properties of solutions to the two equations.

Property	Wave equation	Heat equation
Speed of propogation	Finite	Infinite
Smoothing	No	Yes
Supports a maximum principle	No	Yes
Energy	Conserved	Decays
Time reversable	Yes	No

Table 1: Properties of the wave and heat equations.

7.5 The heat equation on a bounded interval

We will conclude our investigation of the heat equation by considering solutions defined on a bounded interval. More precisely, we want to find $u\colon [0,\ell] \times [0,\infty) \to \mathbf{R}$ such that

$$\begin{cases} \partial_t u(x,t) - \partial_{xx} u(x,t) = 0 & \text{for } x \in (0,\ell) \text{ and } t \in (0,\infty); \\ u(x,0) = \phi(x) & \text{for } x \in [0,\ell]; \\ u(0,t) = 0 \quad \text{and} \quad u(\ell,t) = 0 & \text{for } t > 0. \end{cases} \tag{7.4}$$

When we considered a similar domain for the wave equation we used ideas about reflection in order to construct a solution. Such a method would work well here, but we will try another method, separation of variables, which we have already applied to Laplace's equation.

Suppose that a solution to (7.4) can be written in the form

$$u(x,t) = X(x)T(t).$$

Substututing this into the heat equation, we see that

$$X(x)T'(t) - X''(x)T(t) = 0$$

so, dividing by $X(x)T(t)$, we see that

$$\frac{T'(t)}{T(t)} = \frac{X''(x)}{X(x)}$$

which must be independent of x and t, so equal to $-\lambda$, say. This gives us two ODEs to solve, the first is

$$X''(x) + \lambda X(x) = 0 \quad \text{for } x \in [0,\ell], \text{ and } \quad X(0) = 0 \text{ and } X(\ell) = 0 \tag{7.5}$$

so a calculation shows that we must have $\lambda = (k\pi/\ell)^2$ and $X(x) = A\sin(k\pi x/\ell)$ for a constant A and $k \in \mathbf{N}$. The second equation is

$$T'(t) + \lambda T(t) = 0 \quad \text{for } t > 0$$

and a calculation shows that we must have $T(t) = Be^{-\lambda t} = Be^{-(k\pi/\ell)^2 t}$ for a constant B and $k \in \mathbf{N}$. By taking linear combinations of such solutions and we obtain

$$u(x,t) = \sum_{k=1}^{\infty} A_k e^{-(k\pi/\ell)^2 t} \sin(k\pi x/\ell). \tag{7.6}$$

If the sum $\sum_k |A_k|$ converges, then the partial sums

$$u_n(x,t) = \sum_{k=1}^{n} A_k e^{-(k\pi/\ell)^2 t} \sin(k\pi x/\ell)$$

of (7.6) converge uniformly for $x \in (0,\ell)$ and $t \geq 0$, and u will be a continuous function. Moreover for each $\delta > 0$ even the derivatives of the partial sums converge uniformly for $x \in (0,\ell)$ and $t \geq \delta$ provided $\sum_k |A_k| < \infty$, so one can interchange differentiation with the infinite sum to conclude that (7.6) will solve the heat equation and the boundary conditions $u(0,t) = u(\ell,t) = 0$. To ensure the initial condition is satisfied, we require

$$\phi(x) = u(x,0) = \sum_{k=1}^{\infty} A_k \sin(k\pi x/\ell).$$

Thus we require that ϕ can be expressed as a Fourier sine series. This is certainly possible if ϕ is differentiable (although we will not prove this here). In this case, the coefficients are given by

$$A_k = \frac{2}{\ell} \int_0^{\ell} \phi(x) \sin(k\pi x/\ell) dx.$$

8 Numerical analysis

In the preceding sections we have computed explicit formulae for solutions to PDEs in several particular situations. However, in many situations it is not always possible to find such explicit formulae or, even when it is possible, they may prove to be so complicated that they are not practical to use.

The aim of this section is to come up with a scheme that will produce an approximate solution to a PDE together with its boundary/initial conditions by carrying out a finite number of arithmetic operations. Such a scheme could then be implemented by a computer.

Care must be taking when devising such a scheme. We will have to check that any proposed scheme does indeed approximate the solution we are looking for. Below we will see an example of what at first appears to be a reasonable scheme that produces an 'approximation' which is very far from the true solution.

Here we will illustrate the most important methods and techniques using simple equations as examples.

8.1 Finite differences

The notion of a limit is central to the notion of a derivative. However, we cannot compute a limit in a finite number of arithmetic operations, so we must find a suitable replacement. One naturally possibility is that of *finite differences*.

Consider a function $u\colon \mathbf{R} \to \mathbf{R}$ of one variable. We first choose a collection of points x_j from the functions domain $\mathbf{R}$. We can do this by first choosing a *mesh size* δx and then defining $x_j = j(\delta x)$. We can then denote

$$u_j = u(x_j).$$

We have three standard approximations for the first derivative $u'(x_j)$.

$$\text{The backward difference:} \quad \frac{u_j - u_{j-1}}{\delta x}.$$
$$\text{The forward difference:} \quad \frac{u_{j+1} - u_j}{\delta x}.$$
$$\text{The centred difference:} \quad \frac{u_{j+1} - u_{j-1}}{2\delta x}.$$

They are approximations in the sense that the difference between them and the true value of $u'(x_j)$ is smaller the smaller δx is. This can be proved using the Taylor expansion for u. If $u \in C^4(\mathbf{R})$ then

$$u(x+h) = u(x) + u'(x)h + \frac{u''(x)}{2}h^2 + \frac{u'''(x)}{6}h^3 + O(h^4). \tag{8.1}$$

Taking $x = x_j$ and $h = -\delta x$ we see that

$$u'(x_j) = \frac{u_j - u_{j-1}}{\delta x} + O(\delta x),$$

taking $x = x_j$ and $h = \delta x$ we see

$$u'(x_j) = \frac{u_{j+1} - u_j}{\delta x} + O(\delta x), \tag{8.2}$$

and finally taking the difference of (8.1) with $x = x_j$ and $h = \delta x$, and $x = x_j$ and $h = -\delta x$ we see that

$$u'(x_j) = \frac{u_{j+1} - u_{j-2}}{2(\delta x)} + O((\delta x)^2). \tag{8.3}$$

Adding the same two expressions from (8.1) gives us

$$u''(x_j) = \frac{u_{j+1} - 2u_j + u_{j-1}}{(\delta x)^2} + O((\delta x)^2), \tag{8.4}$$

which motivates the following approximation for the second derivative $u''(x_j)$:

$$\text{The centred second difference:} \quad \frac{u_{j+1} - 2u_j + u_{j-1}}{(\delta x)^2}.$$

We will of course be interested in functions of more than one variable. In particular if we have a function u of two variables x and t, we choose mesh sizes δx and δt for each variable. We write

$$u(j(\delta x), n(\delta t)) = u_j^n.$$

Then we can approximate $\partial_t u(j(\delta x), n(\delta t))$ by, for example, the forward difference

$$\frac{u_j^{n+1} - u_j^n}{\delta t}.$$

Similarly, the forward difference for $\partial_x u(j(\delta x), n(\delta t))$ is

$$\frac{u_{j+1}^n - u_j^n}{\delta x},$$

and so on.

8.2 Approximating solutions to the heat equation

8.2.1 An unstable scheme

We begin with what appears to be a simple problem. Let's use the above approximations to produce a scheme for finding approximate solutions to (7.4), the heat equation on a bounded domain with the initial condition $u(x,0) = \phi(x)$. We can use a forward difference to approximate u_t and a centred difference to approximate u_{xx}. Then the PDE is replaced by the difference equation

$$\frac{u_j^{n+1} - u_j^n}{\delta t} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\delta x)^2}. \tag{8.5}$$

Choose a small value of δx so that $\{x_j\}_{j=0}^J$ is a mesh over the interval $[0, \ell]$ with $x_j = j(\delta x)$ and such that $x_J = \ell$ and set $\delta t = (\delta x)^2$. The equation becomes

$$u_j^{n+1} - u_j^n = u_{j+1}^n - 2u_j^n + u_{j-1}^n$$

so

$$u_j^{n+1} = u_{j+1}^n - u_j^n + u_{j-1}^n. \tag{8.6}$$

Now the initial data provides the values u_j^0 for all $j = 0, 1, \ldots, J$, since we can impose that $u_j^0 = \phi(x_j)$. Furthermore, the boundary conditions lead us to set $u_0^n = u_J^n = 0$ for all $n = 1, 2, \ldots$. Then (8.6) can be used to obtain first u_j^1 for all j, then u_j^2 for all j and inductively all u_j^n for all j and n.

Let's implement this scheme with some simple initial data. For example, let's suppose $\ell = 4$, $\delta x = 0.5$ and $u_4^0 = \phi(2) = 1$ and $u_j^0 = \phi(x_j) = 0$ for $j \neq 4$. Then we can compute the values u_j^n as in Table 2.

	$j=0$	$j=1$	$j=2$	$j=3$	$j=4$	$j=5$	$j=6$	$j=7$	$j=8$
$n=0$	0	0	0	0	1	0	0	0	0
$n=1$	0	0	0	1	-1	1	0	0	0
$n=2$	0	0	1	-2	3	-2	1	0	0
$n=3$	0	1	-3	6	-7	6	-3	1	0
$n=4$	0	-4	10	-16	19	-16	10	-4	0
$n=5$	0	14	-30	45	-51	45	-30	14	0

Table 2: Some values of u_j^n computed via (8.6) together with the initial and boundary conditions.

Take a look at Table 2. Does anything appear to have gone wrong? Observe that $|\phi(x)| \leq 1$ for all x but we have computed $u_0^5 = -51$. If we compare the solution $\{u_j^n\}_{j,n}$ of our numerical scheme (8.6) to what Theorem 7.1 says about solutions to the heat equation, we see that our scheme has not produced something close to the true solution.

In the next section we will investigate what has gone wrong and fix it to produce a much better scheme.

8.2.2 A stability condition

We will now investigate why our scheme (8.6) failed. The problem is not easy to spot, although there are subtle clues to what has gone wrong in the form of (8.6). Looking at Table 2, we see that the values of u_j^n oscillate between positive and negative values; this property originates in the fact that (8.6) contains negative coefficients. Let us return to our derivation of (8.6). Above we set $\delta t = (\delta x)^2$ without much thought, but let's repeat the calculation without this assumption. This time we set

$$s = \frac{\delta t}{(\delta x)^2}.$$

Substituting this in (8.5) we obtain

$$u_j^{n+1} = (u_{j+1}^n + u_{j-1}^n)s + (1 - 2s)u_j^n \tag{8.7}$$

To investigate the stability of (8.7), let's further investigate its solution. We can consider the scheme (8.7) together with the initial condition $u_j^0 = \phi(x_j)$ for all $j = 1, 2, \ldots, J$ and boundary conditions $u_0^n = u_J^n = 0$ for all $n = 1, 2, \ldots$. It is not too hard to see that this determines unique values for all u_j^n for $j = 1, 2, \ldots, J$ and $n = 1, 2, \ldots$. Let's now show that these values can be decomposed as

$$u_j^n = X_j T_n.$$

This anzats is the discrete form of separation of variables, that we employed in Section 7.5 for the actual heat equation. Given the method worked for the actual equation, there's good reason to hope it will work for the discrete approximation (8.5). Substituting this anzats in (8.7), we obtain

$$\frac{T_{n+1}}{T_n} = 1 - 2s + s\frac{X_{j+1} + X_{j-1}}{X_j}. \tag{8.8}$$

We argue as usual that both sides must be a constant ξ independent of j and n. Therefore, $T_{n+1} = \xi T_n$ and so, by induction,

$$T_n = \xi^n T_0.$$

At this point we can see that if our numerical approximation of a solution to the heat equation is not going to grow as $n(\delta x) = t \to \infty$, which would contradict the maximum principle (see Theorem 7.1), then we require $|\xi| \leq 1$. However, to determine what ξ is we must look at the right hand side of (8.8).

We have

$$s\frac{X_{j+1} + X_{j-1}}{X_j} + 1 - 2s = \xi. \tag{8.9}$$

To find a solution of this, we guess that because when we solved the heat equation in Section 7.5 the corresponding equation (7.5) was a second order ODE, this should be a discrete form of a second order ODE. Consequently, it is reasonable to guess solutions to (8.9) are of the form

$$X_j = A\cos(j\theta) + B\sin(j\theta),$$

for constants A, B and θ. The boundary condition $u_0^n = 0$ for all $n = 1, 2, \ldots$ implies $A = 0$ and we are free to choose $B = 1$ as we can absorb any constant in T_n. The condition $u_J^n = 0$ for all $n = 1, 2, \ldots$ implies $\sin(J\theta) = 0$ and so $J\theta = k\pi$ for some fixed $k \in \mathbf{N}$. But we know that $J = \ell/\delta x$, so $\theta = k\pi\delta x/\ell$ and

$$X_j = \sin(jk\pi(\delta x)/\ell).$$

Substituting this in (8.9) we have

$$s\frac{\sin((j+1)k\pi(\delta x)/\ell) + \sin((j-1)k\pi(\delta x)/\ell)}{\sin(jk\pi(\delta x)/\ell)} + 1 - 2s = \xi$$

which simplifies to

$$\xi = \xi(k) = 1 - 2s(1 - \cos(k\pi(\delta x)/\ell)). \tag{8.10}$$

Thus, it is easy to see that $1 - 4s \leq |\xi| \leq 1$, so we can only guarantee that $|\xi(k)| \leq 1$ if

$$\frac{\delta t}{(\delta x)^2} = s \leq \frac{1}{2}. \tag{8.11}$$

The condition (8.11) is a stability condition for the numerical scheme (8.7) — it ensures the values we obtain will not oscillate widely as they did in Section 8.2.1. In Section 8.2.4 we will provide an alternative justification that (8.11) is in some sense a stability condition—this takes the form of a maximum principle (Theorem 8.1).

We now turn our attention to motivating that the numerical scheme (8.7) provides a geniune approximation to the solution of (7.4) for small δx. This will also be proved rigourously in Section 8.2.4. Our calculations above show that the solution to the difference scheme (8.7) together with the boundary conditions is

$$u_j^n = \sum_{k=-\infty}^{\infty} B_k \xi(k)^n \sin(jk\pi(\delta x)/\ell)$$

Comparing this to (7.6), we see that we need to justify that, for $n(\delta t) = t$ fixed,

$$\xi(k)^n \to e^{-(k\pi/\ell)^2 t}$$

as $\delta t \to 0$ and $n \to \infty$. Expanding (8.10) as a Taylor series justifies the approximation

$$\xi(k) \approx 1 - s\left(\frac{(k\pi(\delta x)/\ell)^2}{2!}\right) = 1 - \left(\frac{k\pi}{\ell}\right)^2 \delta t.$$

Raising this to the n-th power we have

$$\left(1 - \left(\frac{k\pi}{\ell}\right)^2 \delta t\right)^n = \left(1 - \left(\frac{k\pi}{\ell}\right)^2 \frac{n\delta t}{n}\right)^n = \left(1 - \left(\frac{k\pi}{\ell}\right)^2 \frac{t}{n}\right)^n \approx e^{-(k\pi/\ell)^2 t},$$

as desired. Of course, this is far from a rigorous proof that our numerical scheme approximates the solution, but it certainly provides some encouraging evidence.

8.2.3 The Crank-Nicolson Scheme

Although our choice of scheme (8.5) seemed quite natural, it was nevertheless somewhat arbitrary. For example, given that we used the forward difference $(u_j^{n+1} - u_j^n)/(\delta t)$ to approximate u_t there is no particular reason to use the centred difference

$$\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\delta x)^2}$$

evaluated at time step n verses the centred difference

$$\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\delta x)^2}$$

evaluated at time step $n+1$ to approximate u_{xx}. Indeed, here we will consider a mix of the two: for a fixed $\theta \in [0,1]$ we approximate u_{xx} by

$$(1-\theta)\left(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\delta x)^2}\right) + \theta\left(\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\delta x)^2}\right)$$

and then arrive at a replacement for (8.5)

$$\frac{u_j^{n+1} - u_j^n}{\delta t} = (1-\theta)\left(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\delta x)^2}\right) + \theta\left(\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\delta x)^2}\right) \tag{8.12}$$

for approximating the heat equation. In the particular case $\theta = 0$, (8.12) reduces to our old scheme (8.5), and in the case $\theta = 1/2$, the scheme is called the *Crank-Nicolson scheme*. In contrast to (8.5) we cannot rewrite (8.12) as we did in (8.6), which gave u_j^{n+1} explicitly as an expression involving all the earlier values $(u_j^n)_j$. Instead we obtain a system of linear equations for $(u_j^{n+1})_j$ in terms of the earlier values $(u_j^n)_j$ which must be solved. This is certainly a disadvantage, but let us now motivate why the scheme may be advantageous in another respect.

Analogously to (8.10), we can investigate the issue of stability by assuming a separated solution of the form

$$u_j^n = e^{ik(\delta x)j}\xi(k)^n,$$

where, as before, k could be chosen in combination with a multiplicative constant so that the solution automatically satisfies the zero boundary conditions—but let us not do that just now. From this assumption we can calculate that

$$\xi(k) = \frac{1 - 2(1-\theta)s(1-\cos(k\delta x)}{1 + 2\theta s(1-\cos(k\delta x))}$$

where $s = \delta t/(\delta x)^2$ and we once again look to ensure $|\xi(k)| \leq 1$ so that the solution does not grow for large n. It is easy to check that

$$\xi(k) = 1 - \frac{2s(1-\cos(k\delta x))}{1+2\theta s(1-\cos(k\delta x))}$$

so we always have $\xi(k) \leq 1$ and the condition $\xi(k) \geq -1$ requires

$$s(1-2\theta)(1-\cos(k\delta x)) \leq 1.$$

Since $1-\cos(k\delta x) \leq 2$, this certainly holds if $s(1-2\theta) \leq 1/2$, which is the case if either

$$\frac{1}{2} \leq \theta \leq 1 \tag{8.13}$$

or

$$0 \leq \theta < \frac{1}{2} \quad \text{and} \quad s \leq \frac{1}{2(1-2\theta)}. \tag{8.14}$$

Thus, at least from our preliminary calculations, it appears that (8.14) provides us with a stability condition on s when $\theta < 1/2$, but for $\theta \geq 1/2$, from (8.13) we conclude that the scheme (8.12) appears to be stable regardless of the value of s.

8.2.4 A discrete maximal principle and convergence of (8.7) to the continuous solution

We now return to our numerical scheme (8.7). A solution to this discrete scheme shares some properties with its continuous analogue. In particular it satisfies a maximum principle.

Theorem 8.1 (A Discrete Maximum Principle)**.** *Let $J \in \mathbf{N}$ and $0 < s \leq 1/2$. Suppose that the numbers u_j^n, indexed by $j = 0, 1, 2, \ldots, J$ and $n = 0, 1, 2, \ldots$, satisfy* (8.7)*. Then*

$$\max_{j=1,\ldots,J-1} |u_j^n| \leq \max_{j=0,\ldots,J} |u_j^{n-1}|. \tag{8.15}$$

for each integer $n \geq 1$. As a consequence

$$\sup_{j=0,\ldots,J;n=1,2,\ldots} |u_j^n| \leq \max\left\{ \max_{j=1,\ldots,J-1} |u_j^0|, \sup_{n=0,1,\ldots} |u_0^n|, \sup_{n=0,1,\ldots} |u_J^n| \right\}. \tag{8.16}$$

Proof. Since $0 < s \leq 1/2$, by (8.7) we have

$$\begin{aligned} |u_j^n| &\leq |u_{j+1}^{n-1} + u_{j-1}^{n-1}|s + (1-2s)|u_j^{n-1}| \\ &\leq 2s \max_{k=0,\ldots,J} |u_k^{n-1}| + (1-2s) \max_{k=0,\ldots,J} |u_k^{n-1}| \\ &\leq \max_{k=0,\ldots,J} |u_k^{n-1}| \end{aligned}$$

for $j = 1, \ldots, J-1$, proving (8.15). Consequently

$$|u_j^n| \leq \max_{k=0,\ldots,J} |u_k^{n-1}| \leq \max\left\{ \max_{k=1,\ldots,J-1} |u_k^{n-1}|, \sup_{m=0,1,\ldots} |u_0^m|, \sup_{m=0,1,\ldots} |u_J^m| \right\}$$

for $j = 1, \ldots, J-1$, and (8.16) follows by induction. □

Observe that the proof fails if $s \geq 1/2$, and it is exactly because the terms on the right-hand side of (8.6) have different signs. It is then that there is a possibility for oscillations to occur.

The maximum principle above seems like a natural tool to help prove that the scheme (8.7) produces a close approximation to the continuous solution u to (7.4) for sufficiently small δx and $s \leq 1/2$. Here we present a proof of this, although it requires that we first generalise the result above.

Recall that we for some $J \in \mathbf{N}$ we defined a mesh on $[0,\ell]$ which consisted of the points $x_j = j(\delta x)$ $(j = 0, 1, 2, \dots, J)$ where $\delta x = \ell/J$. We also defined mesh points $t_n = n(\delta t)$ $(n = 0, 1, 2, \dots)$ in the t-variable where

$$\delta t := s(\delta x)^2 = \frac{s\ell}{J}$$

for a given ratio s. The set of points $\{(x_j, t_n) \,|\, j = 0, 1, 2, \dots, J \text{ and } n = 0, 1, 2, \dots\}$ form a grid on the set $[0,\ell] \times [0,\infty)$. For each $\phi\colon [0,\ell] \to \mathbf{R}$ our numerical scheme

$$u_j^{n+1} = (u_{j+1}^n + u_{j-1}^n)s + (1-2s)u_j^n \tag{8.7}$$

produces values u_j^n for each $j = 1, 2, 3, \dots, J-1$ and $n = 1, 2, 3, \dots$, provided we set

$$u_j^0 = \phi(x_j) \text{ for } j = 1, 2, 3, \dots, J-1 \text{ and } u_0^n = u_J^n = 0 \text{ for } n = 0, 1, 2, \dots. \tag{8.17}$$

We now define

$$w_j^n = u(x_j, t_n) - u_j^n \tag{8.18}$$

where u is the solution of (7.4) and u_j^n the solution of the numerical scheme (8.7) and (8.17). Given that u is a solution to the heat equation, w_j^n will satisfy

$$w_j^{n+1} = (w_{j+1}^n + w_{j-1}^n)s + (1-2s)w_j^n + f_j^n \tag{8.19}$$

where f_j^n are the errors between the finite differences of u and derivatives estimated in Section 8.1. Indeed for the solution u to (7.4) we compute

$$\begin{aligned} u(x_j, t_{n-1}) - u(x_j, t_n) &= (\delta t)\partial_t u(x_j, t_n) + O(\delta t) \\ &= (\delta t)\partial_{xx} u(x_j, t_n) + O(\delta t) \\ &= (\delta t)\frac{u(x_{j-1}, t_n) - 2u(x_j, t_n) + u(x_{j+1}, t_n)}{(\delta x)^2} + O((\delta t)(\delta x)^2) \\ &= s(u(x_{j-1}, t_n) - 2u(x_j, t_n) + u(x_{j+1}, t_n)) + O((\delta t)(\delta x)^2) \end{aligned}$$

using (8.2) and (8.4). From this and the fact that u_j^n satisfy (8.7) we conclude that w_j^n satisfy (8.19) with

$$|f_j^n| \le C(\delta t)(\delta x)^2 = \frac{C(\delta t)\ell^2}{J^2} \tag{8.20}$$

for some constant C that only depends on the C^4-norm of u. It is even possible to show that C only need depend on the C^4-norm of the initial data ϕ—compare with exercise 10.2b.

In the hope of showing w_j^n will be small for small mesh sizes we prove the following variation on Theorem 8.1.

Theorem 8.2. *Let $J \in \mathbf{N}$, $A > 0$ and $0 < s \le 1/2$. Suppose that the numbers f_j^n satsifying $|f_j^n| \le A$ for each $j = 0, 1, 2, \dots, J$ and $n = 0, 1, 2, \dots$ are given and the numbers w_j^n, also indexed by $j = 0, 1, 2, \dots, J$ and $n = 0, 1, 2, \dots$, satisfy (8.19) and $w_0^n = w_J^n = 0$ for $n = 0, 1, 2, \dots$. Then*

$$|w_j^n| \le \max_{k=1,\dots,J-1} |w_k^0| + nA \tag{8.21}$$

for integers $j = 1, 2, 3, \dots, J-1$ and $n \ge 1$.

Proof. Since $0 < s \le 1/2$, by (8.19) we have

$$\begin{aligned} |u_j^n| &\le |u_{j+1}^{n-1} + u_{j-1}^{n-1}|s + (1-2s)|u_j^{n-1}| + |f_j^{n-1}| \\ &\le 2s \max_{k=0,\dots,J} |u_k^{n-1}| + (1-2s) \max_{k=0,\dots,J} |u_k^{n-1}| + A \\ &\le \max_{k=0,\dots,J} |u_k^{n-1}| + A \end{aligned}$$

for integers $j = 1, 2, 3, \dots, J-1$ and $n \ge 1$. Since $u_0^{n-1} = u_J^{n-1} = 0$,

$$|u_j^n| \le \max_{k=1,\dots,J-1} |u_k^{n-1}| + A$$

and (8.21) follows by induction. □

Observe that w_j^n from (8.18) satisfy all the hypotheses of Theorem 8.2, even $w_0^n = w_J^n = 0$ for all $n = 0, 1, 2, \ldots$, and $w_j^0 = 0$ for all $j = 1, 2, 3, \ldots, J-1$ so Theorem 8.2 implies that

$$\max_{j=1,\ldots,J-1;n=1,\ldots} |u(x_j, t_n) - u_j^n| = \max_{j=1,\ldots,J-1;n=1,\ldots} |w_j^n| \leq \frac{Cn(\delta t)\ell^2}{J^2}$$

by (8.21) and (8.20). Therefore for a fixed time $T > 0$ we can ensure that

$$\max_{j=1,\ldots,J-1;n=1,\ldots} |u(x_j, t_n) - u_j^n| \leq \frac{CT\ell^2}{J^2}$$

provided $t_j \leq T$. Thus, for each $\varepsilon > 0$ and $T > 0$, we have succeeded in proving

$$\max_{j=1,\ldots,J-1;n=1,\ldots} |u(x_j, t_n) - u_j^n| \leq \varepsilon$$

for $t_n \leq T$ provided J is chosen larger than $\ell\sqrt{CT}/\varepsilon$ (or equivalently, δx is chosen smaller than $\varepsilon/\sqrt{CT}$ and δt smaller than $s\varepsilon^2/(CT)$), were C is a constant that can be chosen depending only on the C^4-norm of the initial data ϕ.

8.3 Approximations of Laplace's equation

8.3.1 A discrete mean value property

Let us now study Laplace's equation in two dimensions. We begin just as before by defining grid points $x_j = j(\delta x)$ and $y_k = k(\delta y)$ for fixed δx and δy, and $j, k \in \mathbf{Z}$. We can then approximate the Laplace operator $\Delta = \partial_{xx} + \partial_{yy}$ by the sum of the centred differences. So, with $u_{j,k} = u(x_j, y_k)$, Laplace's equation $\Delta u = 0$ is approximated as

$$\frac{u_{j+1,k} - 2u_{j,k} + u_{j-1,k}}{(\delta x)^2} + \frac{u_{j,k+1} - 2u_{j,k} + u_{j,k-1}}{(\delta y)^2} = 0.$$

If we choose $\delta x = \delta y$ we can simplify this to

$$u_{j,k} = \frac{1}{4}\left(u_{j+1,k} + u_{j-1,k} + u_{j,k+1} + u_{j,k-1}\right). \tag{8.22}$$

Thus $u_{j,k}$ is the average of the values at the four adjacent points — that is, a discrete version of the mean value property (Theorem 5.3) holds![9] Just as is the continuous case, we can use this to prove a strong maximum principle.

Given $(j, k) \in \mathbf{Z}^2$ we call $(j+1, k)$, $(j-1, k)$, $(j, k+1)$ and $(j, k-1)$ the *adjacent points* of (j, k). Given $D \subseteq \mathbf{Z}^2$, we say a point in D is an *interior point* of D if its adjacent points are also contained in D and a point is a *boundary point* if at least one of it's adjacent points is not contained in D. The set of all boundary points of D is denoted ∂D. We say $D \subseteq \mathbf{Z}^2$ is *discretely connected* if, for each pair of points $p, q \in D$, there exists $N \in \mathbf{N}$ and interior points p_i for $i = 1, \ldots, N$ such that p_{i+1} is an adjacent point of p_i for $i = 0, \ldots, N$ with $p_0 = p$ and $p_{N+1} = q$.

Theorem 8.3 (Discrete strong maximum principle)**.** *Suppose $D \subseteq \mathbf{Z}^2$ is discretely connected and $u\colon D \to \mathbf{R}$ satisfies* (8.22) *(with $u(j, k) = u_{j,k}$) at each interior point (j, k). Then, if u attains either a maximum or minimum at an interior point of D, u is constant.*

Again, just like the continuous case, this theorem can be used to prove the uniqueness of a solution $(u_{j,k})_{j,k}$ and in this case, the uniqueness of solutions also proves existence.

[9] An equation involving finite differences is often refereed to as a *discrete* version, and its original form, involving either derivatives or integrals (and thus implicitly limits) is refereed to as the *continuous* version. Many ideas in calculus can be formulated in both continuous and discrete versions. For example, summation by parts is the discrete analogue of integration by parts.

Theorem 8.4. *Suppose $D \subseteq \mathbf{Z}^2$ is discretely connected and we are given an $f\colon \partial D \to \mathbf{R}$. Then there exists a unique $u\colon D \to \mathbf{R}$ that satisfies (8.22) (with $u(j,k) = u_{j,k}$) at each interior point (j,k) and $u(j,k) = f(j,k)$ for each $(j,k) \in \partial D$.*

Proof. Suppose we have two functions $v^1, v^2\colon D \to \mathbf{R}$ satisfying the hypothesis of the theorem. Then $u_{j,k} = v^2(j,k) - v^1(j,k)$ satisfies (8.22) at each interior point (j,k) and $u_{j,k} = 0$ for each $(j,k) \in \partial D$. By Theorem 8.3 $u_{j,k} = 0$ for all $(j,k) \in D$ which implies $v^1 = v^2$ and we have proved uniqueness.

To prove existence, let N denote the number of interior points in D. Observe that (8.22) gives us N linear equations in the N unknowns $u_{j,k}$, and this system can be written in the form $A\mathbf{v} = \mathbf{f}$, where A is an $N \times N$ matrix, $\mathbf{v}$ is a vector with the N components $u_{j,k}$, and $\mathbf{f}$ is a vector with elements depending on f such that $\mathbf{f} = \mathbf{0}$ when $f \equiv 0$. By our proof of uniqueness above we have proved that the kernel of the matrix A is trivial. Therefore, by the rank-nullity theorem, the image of A is $\mathbf{R}^N$, so for each $\mathbf{f}$ there exists a solution and we have proved existence. □

8.3.2 The finite element method

So far in this chapter we have found numerical schemes to approximate the solution of differential equations by replacing derivatives with finite differences. It seemed a natural approach, although, as we saw, it also presented some problems. There are, however, other approaches that can also be taken. Once such alternative is called the *finite element method*. The method makes greater use of linear algebra to approximate solutions.

We will study the Dirichlet problem for Poisson's equation:

$$\begin{cases} -\Delta u = f & \text{in } \Omega, \text{ and} \\ u = 0 & \text{on } \partial\Omega. \end{cases} \tag{8.23}$$

First we shall find a convenient way to rewrite the boundary value problem. Let us denote the set of all functions $v \in C^2(\overline{\Omega})$ which also satisfies the boundary condition $v = 0$ on $\partial\Omega$ by $C^2(\overline{\Omega})$. If we multiply both side of the PDE in (8.23) by an arbitrary function $v \in C_0^2(\overline{\Omega})$, integrate over Ω and apply Green's first identity (5.8), we obtain

$$\int_\Omega \nabla u(\mathbf{x}) \cdot \nabla v(\mathbf{x}) d\mathbf{x} = \int_\Omega (-\Delta u)(\mathbf{x}) v(\mathbf{x}) d\mathbf{x} = \int_\Omega f(\mathbf{x}) v(\mathbf{x}) d\mathbf{x}.$$

Interestingly, if we were given a function $u \in C_0^2(\overline{\Omega})$ such that

$$\int_\Omega \nabla u(\mathbf{x}) \cdot \nabla v(\mathbf{x}) d\mathbf{x} = \int_\Omega f(\mathbf{x}) v(\mathbf{x}) d\mathbf{x}. \tag{8.24}$$

for all functions $v \in C_0^2(\overline{\Omega})$, then we could apply Green's first identity again, to conclude

$$\int_\Omega (-\Delta u)(\mathbf{x}) v(\mathbf{x}) d\mathbf{x} = \int_\Omega f(\mathbf{x}) v(\mathbf{x}) d\mathbf{x}.$$

Since v was arbitrary, from here we could conclude that $-\Delta u = f$. Thus, we see that if $u \in C_0^2(\overline{\Omega})$, then (8.23) holds if and only if (8.24) holds for all $v \in C_0^2(\overline{\Omega})$. Observe that the boundary condition in (8.23) holds by definition if $u \in C_0^2(\overline{\Omega})$.

The reformulation (8.24) is useful, as it emphasises the role of the vector space $C_0^2(\overline{\Omega})$. But how does this help us find a numerical solution to (8.23)? The idea is to replace $C_0^2(\overline{\Omega})$ with a finite dimensional vector subspace V of $C_0^2(\overline{\Omega})$. The task then becomes to $u_V \in V$ such that

$$\int_\Omega \nabla u_V(\mathbf{x}) \cdot \nabla v(\mathbf{x}) d\mathbf{x} = \int_\Omega f(\mathbf{x}) v(\mathbf{x}) d\mathbf{x} \tag{8.25}$$

holds for all $v \in V$. If $\{v_1, v_2, \ldots, v_N\}$ is a basis for V, then we can write

$$u_V = \sum_{i=1}^N \alpha_i v_i,$$

$$\sum_{i=1}^{N} \alpha_i \int_\Omega \nabla v_i(\mathbf{x}) \cdot \nabla v_j(\mathbf{x}) d\mathbf{x} = \int_\Omega f(\mathbf{x}) v_j(\mathbf{x}) d\mathbf{x}$$

for each $j = 1, 2, \ldots, N$. Writing $f_k = \int_\Omega f(\mathbf{x}) v_k(\mathbf{x}) d\mathbf{x}$ and $m_{ij} = \int_\Omega \nabla v_i(\mathbf{x}) \cdot \nabla v_j(\mathbf{x}) d\mathbf{x}$, this is just the system of linear equations,

$$\sum_{i=1}^{N} m_{ij} \alpha_i = f_j,$$

which can be easily solved by inverting the matrix $(m_{ij})_{ij}$.

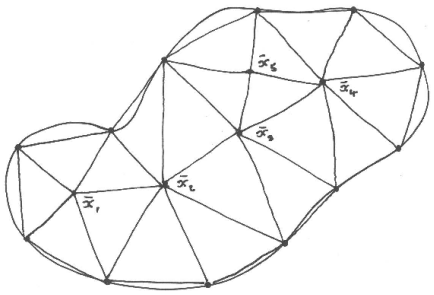


Figure 7: A triangulation of the set Ω with interior vertices labelled $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_5$.

In order to implement these ideas we need to find an explicit finite dimensional vector space V and associated basis. One way to do this is to find a triangulation of Ω. This involves approximating Ω by a union of triangles (see Figure 7). Enumerate the vertices of the triangulation which lie in the interior of Ω by $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ and then, for each $k = 1, 2, \ldots, N$, define a function v_k which is equal to one at $\mathbf{x}_k$, equal to zero at all other vertices, and extended to be linear in each triangle. Thus, each v_k is piecewise linear. It is also easy to check that $\{v_1, v_2, \ldots, v_N\}$ is linear independent, and so $\{v_1, v_2, \ldots, v_N\}$ is a basis for its linear span, which we take as our finite dimensional vector space V.

Strictly speaking, V is not a subspace of $C_0^2(\overline{\Omega})$, but nevertheless it works well.(Explaining why this is okay is beyond the scope of this course, but the idea is that the reformulation (8.24) dispenses with the need to worry about second-order derivatives, and as distributions the first-order derivatives of elements in V are well-behaved.)

9 Schrödinger's equation

The Schrödinger equation describes quantum mechanical phenomena, such as how electrons are distributed around the nucleus of an atom. I have not succeeded in finding a very clear motivation as to why the Schrödinger equation is the correct equation to study, but it appears to be a very good model, which can, for example, reproduce the electron shell structure which underpins chemical reactions. The Schrödinger equation we will study takes the form

$$-i\hbar \partial_t u(\mathbf{x}, t) = \frac{\hbar^2}{2m} \Delta u(\mathbf{x}, t) + V(\mathbf{x}) u(\mathbf{x}, t) \tag{9.1}$$

where $\hbar$ (Plank's constant) and m (the electron's mass) are constants, $x \in \mathbf{R}^3$ is the spatial variable, $t \in \mathbf{R}$ represents time and the function V is a potential, which will depend on the situation being studied. The solution u is usually refereed to as a *wave function* and is connected to the probability distribution for the electron. The probability that an electron is located in a region $E \subset \mathbf{R}^3$ at time t is given by

$$\frac{\int_E |u(\mathbf{x}, t)|^2 dx}{\int_{\mathbf{R}^3} |u(\mathbf{x}, t)|^2 dx}.$$

If we consider electrons in free space, then we take $V \equiv 0$. In this case the equation is similar in form to the heat equation, with the only substantial mathematical difference being the complex constant i. However, this difference is in fact significant and results in solutions behaving more like solutions to the wave equation. Indeed the plane wave function

$$(\mathbf{x}, t) \mapsto e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}$$

solves (6.10) provided $|\mathbf{k}| = \omega$, but also solves (9.1) (with $V \equiv 0$) if $|\mathbf{k}|^2\hbar/2m = \omega$.

In the following two sections we study two examples of V where we can solve (9.1) explicitly. The first is a one dimensional toy model analogous to modelling the motion of a spring in classical mechanics, the second models the hydrogen atom and enables us to derive the electron orbitals alluded to above and observed in experiments.

9.1 The harmonic oscillator

We begin with a one dimensional model analogous to that for a spring in classical mechanics. In classical mechanics, Hooke's Law says that the force exerted by a spring is proportional to the length it is compressed or extended. Thus the potential energy contained in the spring is proportional to the length squared. Thus we have a cheap and cheerful motivation for studying a one dimensional version of (9.1) with $V(x) \equiv -x^2$. Choosing the convenient values $\hbar = 1$ and $m = 1/2$ for the (largely irrelevant) constants, we have

$$-i\partial_t u(x,t) = \partial_{xx} u(x,t) - x^2 u(x,t) \tag{9.2}$$

for $x, t \in \mathbf{R}$.

We will search for solutions by separating variables: thus we search for solutions of the form $u(x,t) = v(x)T(t)$. This means we can rewrite (9.2) as

$$-i\frac{T'(t)}{T(t)} = \frac{v''(x) - x^2}{v(x)} = -\lambda$$

for some constant λ. It is thus easy to solve for T, which must be $T(t) = Ae^{-i\lambda t}$ for some constant A. From this we see that any solutions we obtain will be periodic in time.

To find v we are required to solve

$$v''(x) + (\lambda - x^2)v(x) = 0, \tag{9.3}$$

which is hard, not least because the coefficients depend on x. However, in the case $\lambda = 1$ we can guess a solution: $v(x) = e^{-x^2/2}$. Indeed in that case, $v''(x) = x^2e^{-x^2/2} - e^{-x^2/2} = (x^2 - 1)v(x)$. This motivates us to perform the substitution $v(x) = w(x)e^{-x^2/2}$ in order to help us find solutions for other values of λ. Thus

$$v''(x) = (w''(x) - 2xw'(x) + (x^2 - 1)w(x))e^{-x^2/2} \quad \text{and} \quad (\lambda - x^2)v(x) = (\lambda - x^2)w(x)e^{-x^2/2},$$

so (9.3) becomes

$$w''(x) - 2xw'(x) + (\lambda - 1)w(x) = 0. \tag{9.4}$$

This is called *Hermite's differential equation* and can be solved by assuming the solution is a power series $w(x) = \sum_{k=0}^{\infty} a_k x^k$. Substituting this power series in (9.4) we get

$$\sum_{k=0}^{\infty} k(k-1)a_k x^{k-2} - \sum_{k=0}^{\infty} 2ka_k x^k + (\lambda - 1)\sum_{k=0}^{\infty} a_k x^k = 0.$$

Equating powers of x we see a power series solution must satisfy

$$(k+2)(k+1)a_{k+2} = (2k + 1 - \lambda)a_k \quad \text{for each } k \tag{9.5}$$

and a_0 and a_1 can be chosen arbitrarily. Since (9.3) is linear, we can simplify our analysis by studying separately power series with $a_0 \neq 0$ and $a_1 = 0$, which leads via (9.5) to a_k being zero for all odd k and hence an even solution, and power series with $a_0 = 0$ and $a_1 \neq 0$, which leads via (9.5) to a_k being zero for all even k and hence an odd solution.

An interesting case to consider is when $\lambda = 2n + 1$ for some non-negative integer n. This is interesting because (9.5) implies all subsequent coefficients a_{n+2k} (for positive integers k) will be zero. Thus we have found an infinite number of solutions $w(x)$ to (9.3), which we call *Hermite polynomials* and are denoted $H_n(x)$. See Table 3 for the first few. The non-zero values we choose for a_0 or a_1 (for even and odd values of n, respectively) are of course arbitrary if we are only interesting is solving (9.4). However there are particular choices which are commonly taken by convention. The convention depends on whether you are a physicists or a probabilist. Physicists fix the leading coefficient to be 2^n — this is the choice displayed in Table 3 — while probabilist fix the leading coefficient to be one.

n	λ	a_0	a_1	$H_n(x)$
0	1	1	0	1
1	3	0	2	$2x$
2	5	-2	0	$4x^2 - 2$
3	7	0	-12	$8x^3 - 12x$
4	9	12	0	$16x^4 - 48x^2 + 12$
5	11	0	120	$32x^5 - 160x^3 + 120x$

Table 3: The first six Hermite polynomials.

Finally then, we can write down the solutions we have obtained for (9.2). The functions $v(x) = H_n(x)e^{-x^2/2}$ solve (9.3) with $\lambda = 2n + 1$ and so

$$u_n(x, t) = e^{-i(2n+1)t} H_n(x) e^{-x^2/2}$$

solves (9.2) with $u = u_n$ for each non-negative integer n. The solutions are the quantum mechanical analogue of calculating the motion of a weight hanging on a spring. The constant λ can be interpreted physically as the energy of the solution and moreover one can calculate (although we will not here) that other values of λ do not lead to physically meaningful solutions. Thus we see that the energy λ of the system is quantised and can only take on the values $\lambda = 2n + 1$ for non-negative integers n.

9.2 The hydogen atom

We now solve (9.1) with a potential that models the hydrogen atom, which has a positively charged nucleus at its centre. We take $V(\mathbf{x}) = |\mathbf{x}|^{-1}$ and fix $\hbar = m = 1$ so (9.1) becomes

$$-i\partial_t u(\mathbf{x}, t) = \frac{1}{2}\Delta u(\mathbf{x}, t) + \frac{u(\mathbf{x}, t)}{|\mathbf{x}|}. \tag{9.6}$$

The solutions we construct will give possible wave functions for electrons in a hydrogen atom. Again we separate variables, looking for solutions $u(\mathbf{x}, t) = T(t)v(\mathbf{x})$. We obtain

$$2i\frac{T'(t)}{T(t)} = \frac{-\Delta v(\mathbf{x}) + \frac{2v(\mathbf{x})}{|\mathbf{x}|}}{v(\mathbf{x})} = \lambda.$$

Thus $T(t) = e^{-i\lambda t/2}$ and we also need to solve

$$-\Delta v(\mathbf{x}) + \frac{2v(\mathbf{x})}{|\mathbf{x}|} = \lambda v(\mathbf{x}).$$

If we restict ourselves to radial solutions $v(\mathbf{x}) = R(|\mathbf{x}|)$ we can calculate similarly to as we did in Section 5.3.1 (although we omit the details) that the equation becomes

$$-R''(r) - \frac{2}{r}R'(r) - \frac{2}{r}R(r) = \lambda R(r). \tag{9.7}$$

It turns out there also exist other solutions which are not radially symmetric, but we will satisfy ourselves with radially symmetric ones for now. Physically this radial symmetry corresponds to orbitals which have zero angular momentum. As in Section 9.1, (9.7) is hard to solve as written, so we perform a substitution. We can motivate the substitution as follows. For large r the second two terms on the left-hand side of (9.7) should be small, so the equation is essentially $-R''(r) = \lambda R(r)$. In the case $\lambda < 0$ this has a solution which decays for large r: $R(r) = e^{-\beta r}$ where $\beta = \sqrt{-\lambda}$. For other values of λ the solution does not decay for large r (and thus seems more physically relevant for an electron bound to a nucleus), so we will from here on just consider $\lambda < 0$. Moreover, this argument motivates the substitution $R(r) = (w'(r) - \beta w(r))e^{-\beta r}$, which yields $R'(r) = (w'(r) - \beta w(r))e^{-\beta r}$ and $R''(r) = (w''(r) - 2\beta w'(r) + \beta^2 w(r))e^{-\beta r}$, so (9.7) is transformed to

$$-(w''(r) - 2\beta w'(r) + \beta^2 w(r))e^{-\beta r} - \frac{2}{r}(w'(r) - \beta w(r))e^{-\beta r} - \frac{2}{r}w(r)e^{-\beta r} - \lambda w(r)e^{-\beta r} = 0,$$

which we simplify first to

$$-w''(r) - 2\left(1 - \frac{1}{r}\right)w'(r) - \left(2(\beta - 1)\frac{1}{r}\right)w(r) = 0$$

and finally to

$$\frac{r}{2}w''(r) - \beta r w'(r) + w'(r) + (1 - \beta)w(r) = 0. \tag{9.8}$$

Ignoring the potential problem that the coefficients are zero when $r = 0$, we search for power series solutions to (9.8). That is, we set

$$w(r) = \sum_{k=0}^{\infty} a_k r^k$$

and compute that (9.8) then takes the form

$$\begin{aligned} 0 &= \frac{1}{2}\sum_{k=1}^{\infty} k(k-1)a_k r^{k-1} - \beta\sum_{k=0}^{\infty} k a_k r^k + \sum_{k=1}^{\infty} k a_k r^{k-1} + (1-\beta)\sum_{k=0}^{\infty} a_k r^k \\ &= \frac{1}{2}\sum_{k=1}^{\infty} k(k-1)a_k r^{k-1} - \beta\sum_{k=1}^{\infty}(k-1)a_{k-1} r^{k-1} + \sum_{k=1}^{\infty} k a_k r^{k-1} + (1-\beta)\sum_{k=1}^{\infty} a_{k-1} r^{k-1}. \end{aligned}$$

For each coefficient to vanish we require

$$\frac{k(k+1)}{2}a_k = (\beta k - 1)a_{k-1} \quad \text{for } k = 1, 2, 3, \ldots.$$

If β equals $1/n$ for some positive integer n, the power series terminates and w is a polynomial. Table 4 shows the solutions we obtain for the first few values of n where we take $a_0 = 1$.

n	β	λ	$w(r)$	$R(r)$
1	1	-1	1	e^{-r}
2	1/2	$-1/4$	$1 - \frac{1}{2}r$	$(1 - \frac{1}{2}r)e^{-r/2}$
3	1/3	$-1/9$	$1 - \frac{2}{3}r + \frac{2}{27}r^2$	$(1 - \frac{2}{3}r + \frac{2}{27}r^2)e^{-r/3}$
4	1/4	$-1/16$	$1 - \frac{3}{4}r + \frac{2}{16}r^2 - \frac{1}{192}r^3$	$(1 - \frac{3}{4}r + \frac{2}{16}r^2 - \frac{1}{192}r^3)e^{-r/4}$

Table 4: The first four solutions to (9.8) and (9.7).

Just as in Section 9.1, λ can be interpreted as the energy of the electron shell. Thus we expect the energy levels of electrons in hydrogen to be proportional to $1/n^2$ for integer values of n.[10] This is indeed the case and can be verified experimentally.

[10]Recall we have chosen convenient values for various constants, so the energy will only be correct in units where these choices are the correct values.