1. Review of some fundamental techniques

This first lecture covers some techniques that you have probably already encountered; it is mainly a review. To illustrate the techniques, we use the heat equation with various initial and boundary conditions.

First we consider the initial-value problem on the infinite domain:

$$\begin{aligned} &\theta_t = \kappa\,\theta_{xx}, \quad -\infty < x < +\infty, \quad t > 0 \\ &\theta(x,0) = f(x) \end{aligned} \tag{1}$$

where $f(x)$ is a given function. The boundary conditions are $\theta \to 0$ as $x \to \pm\infty$. In the method of *separation of variables* one seeks solutions in the form

$$\theta(x,t) = F(t)G(x). \tag{2}$$

Then

$$\theta_t = \kappa\,\theta_{xx} \Rightarrow F_t G = \kappa\, F\, G_{xx} \Rightarrow \frac{F_t}{\kappa F} = \frac{G_{xx}}{G} = const \tag{3}$$

By the boundary conditions, this constant must be negative, i.e. $const = -k^2$. Then

$$G = C_1 e^{ikx} + C_2 e^{-ikx} \qquad \text{and} \qquad F = C_3 e^{-k^2 \kappa t}. \tag{4}$$

where C_i are arbitrary constants. From this we conclude that

$$\theta(x,t) = A e^{ikx - k^2 \kappa t} \tag{5}$$

is a solution to the heat equation in the unbounded domain, where A is *any* constant, and k is any *real* constant. The general solution is a superposition of solutions like (5), each with a different A and k. Since k can take any (real) value, this superposition takes the form of an integral,

$$\theta(x,t) = \int_{-\infty}^{+\infty} A(k)\, e^{ikx - k^2 \kappa\, t}\, dk \tag{6}$$

where $A(k)$ is an arbitrary function. To satisfy the initial condition in (1), we choose $A(k)$ to make

$$\theta(x,0) = \int_{-\infty}^{+\infty} A(k)\, e^{ikx}\, dk = f(x). \tag{7}$$

Thus $A(k)$ is the Fourier transform of $f(x)$. Recalling Fourier's theorem—which we prove below—we obtain

$$A(k) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} f(x')\, e^{-ikx'}\, dx'. \tag{8}$$

Thus the solution to the initial value problem (1) is

(9) $$\theta(x,t) = \int_{-\infty}^{+\infty}\left[\frac{1}{2\pi}\int_{-\infty}^{+\infty} f(x')e^{-ikx'}dx'\right]e^{ikx-k^2\kappa t}dk = \int_{-\infty}^{+\infty}\left[\frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{ik(x-x')-k^2\kappa t}dk\right]f(x')dx' .$$

That is,

(10) $$\theta(x,t) = \int_{-\infty}^{+\infty} G(x,x',t)f(x')dx'$$

where

(11) $$G(x,x',t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\cos(k\xi)e^{-k^2\kappa t}dk, \qquad \xi \equiv x - x' .$$

This is an integral which may be looked up in the form,

(12) $$\int_{-\infty}^{+\infty} e^{-ax^2}\cos(bx)dx = \sqrt{\frac{\pi}{a}}\, e^{-b^2/4a} .$$

Thus

(13) $$G(x,x',t) = \frac{1}{\sqrt{4\pi\kappa t}} e^{-(x-x')^2/4\kappa t} .$$

The function $G(x,x',t)$ is called the *Green's function*. Its physical interpretation is this:

(14) $$G(x,x',t) = \theta(x,t) \qquad \text{when} \qquad f(x) = \delta(x - x') .$$

That is, the Green's function is the response to an initial pulse at $x = x'$. Thus the Green's function is *defined* by the problem:

(15) $$\begin{aligned} &\frac{\partial}{\partial t}G(x,x_0,t) = \kappa\frac{\partial^2}{\partial x^2}G(x,x_0,t), \qquad -\infty < x < +\infty,\ t > 0 \\ &G(x,x_0,0) = \delta(x - x_0) \end{aligned}$$

Instead of the method we have followed for solving (1), we could instead use (15) to determine $G(x,x_0,t)$, and then take (10) as the solution of (1). This second method has several advantages:

1. The Green's function offers physical insight. It contains the essence of the heat equation: As t increases, the Green's function flattens and widens, keeping its area the same (conservation of heat).

2. The same $G(x,x_0,t)$ works for any $f(x)$. Thus we need to solve for G only once.

3. We can sometimes manufacture the Green's function for a new problem from the Green's function known from another problem.

As an example of the last property, consider the problem

$$\begin{aligned} &\theta_t = \kappa\,\theta_{xx}, \quad 0 < x < +\infty, \quad t > 0 \\ (16)\qquad &\theta(0,t) = 0, \qquad \theta \to 0 \quad \text{as} \quad x \to \infty \\ &\theta(x,0) = f(x) \end{aligned}$$

on the semi-infinite domain. The problem (16) is clearly equivalent to (1) with $f(x)$ extended as an odd function to negative x. Then the solution of (1) is

(17) $$\theta(x,t) = \int_{-\infty}^{+\infty} G(x-x',t) f(x')\,dx'$$

where G is given by (13), and f is extended to negative x by

(18) $$f(x) = -f(-x).$$

Using (18), (17) can be written

(19) $$\theta(x,t) = \int_{0}^{+\infty} \left[G(x-x',t) - G(x+x',t) \right] f(x')\,dx'.$$

The square brackets in (19) enclose the Green's function of (16). Note that the result (19) might have been guessed directly, using the physical interpretation of the basic Green's function G.

What is the Green's function for (16) with the boundary condition replaced by $\theta_x(0,t) = 0$?

Before going on to more examples, we pause for a proof of

Fourier's theorem. If $f(x) = \int_{-\infty}^{+\infty} F(k) e^{ikx}\,dk$, then $F(k) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} f(x) e^{-ikx}\,dx$.

Alternatively,

(20) $$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{ikx}\,dk.$$

Rough-and-ready proof:

$$\int_{-\infty}^{+\infty} e^{ikx} dk = \int_{-\infty}^{+\infty} \cos kx \; dk + i \int_{-\infty}^{+\infty} \sin kx \; dk \tag{21}$$

However, neither integral makes sense except as a limit. Letting

$$\begin{aligned}\int_{-\infty}^{+\infty} \cos kx \; dk &= \lim_{\varepsilon \to 0} \int_{-\infty}^{+\infty} \cos kx \; e^{-\varepsilon k^2} dk = \lim_{\varepsilon \to 0} \sqrt{\frac{\pi}{\varepsilon}} \, e^{-x^2/4\varepsilon} = 2\pi \, \delta(x) \\ \int_{-\infty}^{+\infty} \sin kx \; dk &= \lim_{\varepsilon \to 0} \int_{-\infty}^{+\infty} \sin kx \; e^{-\varepsilon k^2} dk = 0\end{aligned} \tag{22}$$

we obtain the result. More rigorous proofs are accompanied by hypotheses that $F(k)$ and $f(x)$ vanish sufficiently fast at infinity, making it unnecessary to take the limits.

Fourier analysis in relation to separation of variables

Fourier transformation is more direct than separation of variables. For example, to solve (1) we could introduce the Fourier transforms

$$\theta(x,t) = \int_{-\infty}^{+\infty} \hat{\theta}(k,t) e^{ikx} dk, \qquad f(x) = \int_{-\infty}^{+\infty} \hat{f}(k) e^{ikx} dk. \tag{23}$$

Then the transform of (1) is

$$\frac{\partial}{\partial t} \hat{\theta}(k,t) = -\kappa \, k^2 \hat{\theta}(k,t) \tag{24}$$

with initial condition $\hat{\theta}(k,0) = \hat{f}(k)$. The solution is $\hat{\theta}(k,t) = \hat{f}(k) e^{-\kappa k^2 t}$, so

$$\theta(x,t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \hat{f}(k) e^{ikx - \kappa k^2 t} dk, \tag{25}$$

which is just (9). The Green's function problem (15) could also be solved in this way. (Fourier's theorem tells us that the Fourier transform of $\delta(x)$ is $1/2\pi$.)

One disadvantage of Fourier analysis is that it often fails to be useful if the domain is bounded. In that case, we might still use separation of variables. For example, consider the problem

$$\begin{aligned}&\theta_t = \kappa \, \theta_{xx}, \qquad 0 < x < L \\ &\theta(0,t) = \theta(L,t) = 0 \\ &\theta(x,0) = f(x)\end{aligned} \tag{26}$$

In this case, the hypothesis $\theta(x,t) = F(t)G(x)$ yields $G = A\sin kx + B\cos kx$ as before, but now the boundary conditions imply that B=0 and $k = n\pi / L$ where n=1,2,3... The general solution constructed in this way is

$$\theta(x,t) = \sum_{n=1}^{\infty} A_n e^{-\frac{n^2\pi^2}{L^2}\kappa t} \sin\left(\frac{n\pi x}{L}\right) \tag{27}$$

where A_n is chosen to staisfy $f(x) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi x}{L}\right)$. We find that

$$A_n = \frac{2}{L}\int_0^L f(x)\sin\left(\frac{n\pi x}{L}\right)dx . \tag{28}$$

This is not a Fourier transform, but it is closely related; it is a sine transform. What is the Green's function corresponding to (27-28)?

The experienced applied mathematician would not require separation of variables to identify (26) as a suitable candidate for a sine transform. However, some problems have basic solutions whose forms are very hard to guess beforehand. Separation of variables can often be used to find them. For example, consider the problem

$$\begin{aligned} &\theta_t = \kappa\,\theta_{xx}, \qquad 0 < x < L \\ &\theta(0,t) = \theta_x(L,t) = 0 \\ &\theta(x,0) = f(x) \end{aligned} \tag{29}$$

which differs from (26) by a single boundary condition. In this case separation of variables leads to the basic solution

$$\theta(x,t) = e^{-k_n{}^2\kappa t}\sin(k_n\, x) \tag{30}$$

where

$$k_n = \frac{\pi}{2L}(2n+1). \tag{31}$$

To solve (29) we choose the coefficients in

$$\theta(x,t) = \sum_{n=1}^{\infty} A_n\, e^{-k_n{}^2\kappa t}\sin(k_n\, x) \tag{32}$$

to meet the initial condition. To do this, it helps to recognize that the functions $G_n(x) \equiv \sin(k_n\, x)$ are orthogonal,

$$\int_0^L G_n(x)G_m(x)dx = \frac{L}{2}\delta_{nm}. \tag{33}$$

Thus we might regard separation of variables as a kind of *generalized Fourier analysis*.

When does Fourier analysis fail? Usually when there are nonconstant coefficients. For example, the equation

(34) $$\theta_t = \kappa(x)\theta_{xx}$$

cannot generally be solved by (spatial) Fourier transformation.

When does separation of variables fail? Often when symmetry is lacking. For example,

(35) $$\theta_t = \kappa(x,t)\theta_{xx}$$

cannot be solved by separation of variables unless $\kappa(x,t)=\kappa_1(x)\kappa_2(t)$.

Fourier analysis in relation to Green's functions

These can be viewed as *alternative representations* of the functions in the problem. In the Fourier viewpoint,

(36) $$f(x) = \int_{-\infty}^{+\infty} \hat{f}(k)e^{ikx}dk,$$

and $\hat{f}(k)$ is the amplitude of the basis function e^{ikx}. Each k corresponds to a different basis function. The problem is solved *one basis function at a time*, and the solution is obtained by adding up the results.

In the Green's function viewpoint,

(37) $$f(x) = \int_{-\infty}^{+\infty} f(x_0)\delta(x-x_0)dx_0,$$

and $f(x_0)$ is the amplitude of the basis function $\delta(x-x_0)$. Each x_0 corresponds to a different basis function. Again the problem is solved one basis function at a time.

Both methods clearly rely on the superposition of solutions and hence only apply to linear equations. Note that e^{ikx} are very nonlocal basis functions, whereas $\delta(x-x_0)$ are very local. Thus the two methods represent extremes.

Some more examples of finding one Green's function from another

We continue to let

(38) $$G(x-x_0,t)=\frac{1}{\sqrt{4\pi\kappa t}}e^{-(x-x_0)^2/4\kappa t}$$

denote the basic Green's function for the initial value problem (1) on the infinite domain. Now we consider the infinite-domain problem

(39) $$\begin{aligned}&\theta_t=\kappa\,\theta_{xx}+Q(x,t), \quad -\infty<x<+\infty, \quad t>0\\ &\theta(x,0)=0\end{aligned}$$

with the source $Q(x,t)$. The problem (39) includes (1) as a special case, namely $Q(x,t)=f(x)\,\delta(t)$, suggesting that the solution of (39) is

(40) $$\theta(x,t)=\int_0^t dt_0\int_{-\infty}^{+\infty}dx_0\,Q(x_0,t_0)\,G(x-x_0,t-t_0)\,.$$

It is as if Q lays down a new initial condition at each time. To check (40) we compute

$$\begin{aligned}\theta_t-\kappa\,\theta_{xx}&=\int_0^t dt_0\int_{-\infty}^{+\infty}dx_0\,Q(x_0,t_0)\left[\partial_t-\kappa\partial_{xx}\right]G(x-x_0,t-t_0)+\int_{-\infty}^{+\infty}dx_0\,Q(x_0,t)G(x-x_0,t-t)\\ &=0+\int_{-\infty}^{+\infty}dx_0\,Q(x_0,t)\,\delta(x-x_0)=Q(x,t)\end{aligned}$$

where we have used the properties (15) of G.

Next consider the semi-infinite domain problem with an *inhomogeneous boundary condition*,

(41) $$\begin{aligned}&\theta_t=\kappa\,\theta_{xx}, \quad 0<x<\infty, \quad t>0\\ &\theta(x,0)=0\\ &\theta(0,t)=g(t) \qquad (g(0)=0)\end{aligned}$$

The trick here is to define the new dependent variable

(42) $$w(x,t)\equiv\theta(x,t)-g(t)\,.$$

In terms of w, the problem (41) takes the form

(43) $$\begin{aligned}&w_t=\kappa\,w_{xx}-\dot g(t), \quad 0<x<\infty, \quad t>0\\ &w(x,0)=0\\ &w(0,t)=0\end{aligned}$$

Except for the boundary condition at x=0, (43) has the form of (39) with $Q(x,t)=-\dot g(t)$. We handle the boundary condition by the image method, as before. Thus

$$w(x,t) = \int_0^{t_0} dt_0 \int_0^{\infty} dx_0 \; Q(x_0,t_0)\left[G(x-x_0,t-t_0) - G(x+x_0,t-t_0)\right]$$

$$(44) \qquad \equiv \int_0^{t_0} dt_0 \int_0^{\infty} dx_0 \; Q(x_0,t_0)\hat{G}(x,x_0,t-t_0)$$

$$= -\int_0^{t_0} dt_0 \int_0^{\infty} dx_0 \; \dot{g}(t_0)\hat{G}(x,x_0,t-t_0)$$

We wish to express this in "Green's function form", that is, as an integral involving the given function $g(t)$ rather than its derivative. This suggests that we integrate (44) by parts:

$$(45) \qquad w(x,t) = \left[-g(t_0)\int_0^{\infty} \hat{G}\,dx_0\right]_{t_0=0}^{t_0=t} + \int_0^t dt_0 \; g(t_0)\int_0^{\infty} \frac{\partial \hat{G}}{\partial t_0}\,dx_0 \,.$$

The first term in (45) is

$$(46) \qquad -g(t)\int_0^{\infty} \hat{G}(x,x_0,0)\,dx_0 = -g(t)\,.$$

To do the second term we note that

$$(47) \qquad \frac{\partial \hat{G}}{\partial t_0} = -\frac{\partial \hat{G}}{\partial t} = -\kappa\frac{\partial^2 \hat{G}}{\partial x^2} = -\kappa\frac{\partial^2 \hat{G}}{\partial {x_0}^2}\,.$$

Thus

$$(48) \qquad \int_0^{\infty} \frac{\partial \hat{G}}{\partial t_0}\,dx_0 = -\kappa\int_0^{\infty} \frac{\partial^2 \hat{G}}{\partial {x_0}^2}\,dx_0 = +\kappa\left.\frac{\partial \hat{G}}{\partial x_0}\right|_{x_0=0}$$

Since

$$(49) \qquad \hat{G}(x,x_0,t-t_0) = \frac{1}{\sqrt{4\pi\kappa(t-t_0)}}\left[\exp\left(-\frac{(x-x_0)^2}{4\kappa(t-t_0)}\right) - \exp\left(-\frac{(x+x_0)^2}{4\kappa(t-t_0)}\right)\right]$$

we have

$$(50) \qquad \left.\frac{\partial \hat{G}}{\partial x_0}\right|_{x_0=0} = \frac{1}{\sqrt{4\pi\kappa(t-t_0)}}\,\frac{x}{\kappa(t-t_0)}\,e^{-x^2/4\kappa(t-t_0)}\,.$$

Thus

$$(51) \qquad w(x,t) = -g(t) + \int_0^t dt_0 \; g(t_0)\frac{x}{\sqrt{4\pi\kappa}\,(t-t_0)^{3/2}}e^{-x^2/4\kappa(t-t_0)}$$

and finally

$$(52) \qquad \theta(x,t) = w(x,t) + g(t) = \int_0^t dt_0\, \tilde{G}(x,t-t_0)g(t_0)$$

where

$$(53) \qquad \tilde{G}(x,t-t_0) = \frac{x}{\sqrt{4\pi\kappa}\,(t-t_0)^{3/2}}\, e^{-x^2/4\kappa(t-t_0)}$$

is the Green's function for the problem (41). At what location x is $\theta(x,t)$ most affected by the imposed boundary temperature $\theta(0,t_0)$ at the earlier time t_0? Show that the solution (52-53) actually satisfies the boundary condition $\theta(0,t) = g(t)$.

Similarity (symmetry group) methods

Special solutions to partial differential equations may sometimes be found by methods that amount to guessing the form of the solution based on a symmetry property of the equation. Consider our original problem of determining the basic Green's function (13) from its defining problem (15). With no loss in generality we take $x_0 = 0$. Then the problem is to solve

$$(54) \qquad \frac{\partial G}{\partial t} = \kappa \frac{\partial^2 G}{\partial x^2}$$

with initial condition $G(x,0) = \delta(x)$. For this we use "dimensional analysis." Since the variables have the dimensions

$$(55) \qquad [x] = L, \ [t] = T, \ [\kappa] = L^2/T, \ [G] = 1/L.$$

we guess that

$$(56) \qquad \sqrt{\kappa t}\, G = F\left(\frac{x}{\sqrt{\kappa t}}\right)$$

where F is a function to be determined. That is, we assume that the 2 dimensionless quantities $\sqrt{\kappa t}\, G$ and $x/\sqrt{\kappa t}$ are functionally related. The form (56) is one of several equivalent possibilities. (We discuss the reasoning behind (56) more thoroughly after showing how it can save some work.)

To determine F, we substitute (56) into (54). To simplify the algebra we set κ=1 and then resurrect κ in the final result. From

$$(57) \qquad G = \frac{1}{\sqrt{t}} F\left(\frac{x}{\sqrt{t}}\right)$$

it follows that

(58) $$G_{xx} = \frac{1}{t^{3/2}} F''(\xi), \qquad G_t = -\frac{1}{2t^{3/2}}\left(F + \xi F'(\xi)\right)$$

where

(59) $$\xi \equiv x / \sqrt{t}\ .$$

Substituting (58) into (54) yields the ordinary differential equation

(60) $$2\,F''(\xi) + F(\xi) + \xi\, F'(\xi) = 0,$$

which integrates to

(61) $$2\,F'(\xi) + \xi\, F(\xi) = C\,.$$

By the symmetry of the problem, both terms on the left-hand side of (60) must vanish when ξ=0; hence the constant C=0. Then multiplying (60) by $e^{\xi^2/4}$ and integrating again, we obtain

(62) $$F(\xi) = A e^{-\xi^2/4}$$

where A is another constant. Thus

(63) $$G(x,t) = \frac{A}{\sqrt{t}} e^{-x^2/4t}\,.$$

To determine A we use the "conservation of heat":

(64) $$\int_{-\infty}^{\infty} G(x,t)\; dx = 1$$

which implies that $A = 1/\sqrt{4\pi}$. Then replacing t by κt and x by $x - x_0$ we obtain our previous result.

Now what is the *real* reason behind (56)? That is, how does "dimensional analysis" help us to solve a problem that, from a mathematician's viewpoint, involves only pure numbers? What we are really talking about are the *transformation properties* of the equations. We are using the following property of (54): If

(65) $$x' = \alpha x,\ t' = \beta t,\ \kappa' = \frac{\alpha^2}{\beta}\kappa,\quad G' = \frac{1}{\alpha} G$$

where α and β are arbitrary constants, then the whole problem is the same in the primed variables as in the unprimed variables. That is, the transformation (65) implies that

(66) $$\frac{\partial G'}{\partial t'} = \kappa' \frac{\partial^2 G'}{(\partial x')^2} \qquad \text{and} \qquad G'(x',0) = \delta(x')$$

(in which α and β do not appear). Note the analogy between (65) and (55). The transformation (65) is called the *dimensional group* of the heat equation.

If $\alpha^2 = \beta$, then $\kappa' = \kappa$, and the problem has been transformed into itself. Let $G = F(x,t)$ be the solution to the unprimed problem. Its transformation is

(67) $$\alpha G' = F\left(\frac{x'}{\alpha}, \frac{t'}{\alpha^2}\right).$$

But we know that $G'(x',t')$ is a solution of the same problem. Since the solution is unique, the two solutions must be identical, that is,

(68) $$\frac{1}{\alpha} F\left(\frac{x}{\alpha}, \frac{t}{\alpha^2}\right) = F(x,t).$$

Since (68) holds for arbitrary α, F must take the form

(69) $$F(x,t) = \frac{1}{\sqrt{t}} F\left(\frac{x}{\sqrt{t}}\right)$$

(or an equivalent form such as $F\left(x/\sqrt{t}\right)/x$).

These ideas can be greatly extended. For example, it is a remarkable fact that the transformation

(70) $$\begin{aligned} t' &= t + c \\ x' &= x - 2ct - c^2 \\ \theta' &= \theta \exp\left[cx - c^2 t - c^3/3\right] \end{aligned}$$

(where c is an arbitrary constant) transforms the heat equation into itself. That is,

(71) $$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial x^2} \quad \Rightarrow \quad \frac{\partial \theta'}{\partial t'} = \frac{\partial^2 \theta'}{\partial x'^2}$$

(Once again we set κ=1 with no loss in generality.) This is much less obvious than in the case of (65) and requires laborious computation to check.

The transformation (70) has 2 invariants:

(72) $$x + t^2 = x' + (t')^2$$

and

(73) $$\theta \exp\left[-xt - 2t^3/3\right] = \theta' \exp\left[-x't' - 2(t')^3/3\right].$$

These are the analogs of $x / t^{1/2}$ and $\theta\, t^{1/2}$ in the previous example. Thus any solution that is unaffected by the transformation (70) must take the form

(74) $$\theta = \exp\left[xt + 2t^3 / 3\right] F\left(x + t^2\right)$$

where F is found by substituting (74) into the heat equation to obtain an ordinary differential equation.

How does one find transformations like (70)? By a very elegant method invented by Sophus Lie over a century ago. The method is remarkable in that it can be applied to nonlinear equations as easily as linear ones.

Note that (70), unlike (65), does not preserve the initial condition $\theta(x,0) = \delta(x)$. Thus (74) leads to special solutions of the heat equation that do not include the Green's function.

References. The primary reference for this lecture (on the heat equation) is Kevorkian pp 4-54. An excellent introduction to Lie's theory can be found in

Peter J. Olver *Applications of Lie Groups to Differential Equations*. Springer, 1986.

The appendix to this lecture is my attempt at a brief explanation. Read it only if you wish. It is not an official part of the course.