Nine

Separation of Variables and The Diffusion Equation

9.1 Outline of Lecture

- Separation of variables for the Dirichlet problem
- The separation constant and corresponding solutions
- Incorporating the homogeneous boundary conditions
- Solving the general initial condition problem

9.2 Solving the Diffusion Equation via Separation of Variables

In Lecture 5, we derived the homogeneous Dirichlet problem for the diffusion equation. This equation, also called the *Heat Equation*, governs the heat distribution in a finite metal bar of length π, where we keep the endpoints at a fixed temperature, in our case 0. The initial temperature at time $t = 0$ is given by $f(x)$. We derived the following conditions:

The Dirichlet Problem for the Diffusion Equation
(Homogeneous Boundary Conditions)

$$
\begin{array}{rlll}
 & u_t = \kappa u_{xx} & 0 < x < \pi, t > 0 & \mathbb{DE}: \\
u(0,t) = 0 & u(\pi,t) = 0 & t > 0 & \mathbb{BC}: \\
 & u(x,0) = f(x) & 0 < x < \pi, & \mathbb{IC}:
\end{array}
$$

We saw a few solutions to this system, but we didn't have a systematic way of solving the problem given a particular $f(x)$. In this lecture, we will discuss a method to solve the equation for (essentially) any initial $f(x)$.

9.2.1 A Solution to the Homogeneous Dirichlet Problem

In 1807 Jean Baptiste Joseph Fourier caused a big stir when he managed to solve a problem of heat dispersion using what are now called Fourier series. We will use the method he developed to solve our homogeneous Dirichlet problem.

When solving a differential equation, it is frequently advantageous to first look for special solutions that might be easier to find then the general case. Fourier's first step was to look for solutions in the special form

$$u(x,t) = X(x)T(t). \tag{9.1}$$

Plugging this form into the differential equation $u_t = \kappa u_{xx}$, we get

$$X(x)T'(t) = \kappa X''(x)T(t) \tag{9.2}$$

and dividing by $\kappa X(x)T(t)$ we find

$$\frac{T'(t)}{\kappa T(t)} = \frac{X''(x)}{X(x)}. \tag{9.3}$$

Notice that the left hand side is a function of t alone, while the right is a function of x only. This implies that both sides must indeed be constant! Call this constant $-\lambda$. It is known as the *separation constant*. The reason for the negative sign in front of the λ will be apparent shortly.

Thus we have

$$\frac{T'(t)}{\kappa T(t)} = \frac{X''(x)}{X(x)} = -\lambda. \tag{9.4}$$

We can separate this equation into two equations, one involving only x, one involving only t:

$$\frac{T'(t)}{\kappa T(t)} = -\lambda,$$

and

$$\frac{X''(x)}{X(x)} = -\lambda.$$

Each of these equations is now an ordinary differential equation, and thus we can draw on the theory of ordinary differential equations to solve them. The first equation,

$$T'(t) = -\lambda\kappa T(t)$$

has the solution

$$T(t) = Ce^{-\lambda\kappa t}.$$

Note that we expect the temperature to remain finite as time goes to infinity, and thus the exponent to be negative. Thus λ should be non-negative. (Hence the choice of $-\lambda$ earlier.)

The ordinary differential equation in x,

$$X''(x) = -\lambda X(x), \;\; \lambda \geq 0,$$

has the solution

$$X(x) = A\cos(\sqrt{\lambda}x) + B\sin(\sqrt{\lambda}x)$$

for $\lambda > 0$, and

$$X(x) = Ax + B$$

for $\lambda = 0$.

Putting these back together, we find that

$$\begin{aligned} u(x,t) &= Ce^{-\lambda\kappa t}\left(A\cos(\sqrt{\lambda}x) + B\sin(\sqrt{\lambda}x)\right) & \lambda \geq 0 \\ u(x,t) &= C(Ax+B) & \lambda = 0 \end{aligned} \tag{9.5}$$

solve the diffusion equation, though they do not in general satisfy the boundary or initial conditions.

9.3 Incorporating the homogeneous boundary conditions

We wish $u(x,t)$ to satisfy the homogeneous boundary conditions $u(0,t) = u(\pi,t) = 0$. In the case where $u(x,t) = C(Ax+B)$, this forces $u(x,t) = 0$. This is the trivial solution, and we will thus ignore it from now on.

In the case where

$$u(x,t) = Ce^{-\lambda\kappa t}\left(A\cos(\sqrt{\lambda}x) + B\sin(\sqrt{\lambda}x)\right),$$

$$u(0,t) = Ce^{-\lambda\kappa t}A.$$

Thus to have $u(0,t) = 0$ we must have $A = 0$. Thus

$$u(x,t) = Ce^{-\lambda\kappa t}B\sin(\sqrt{\lambda}x).$$

To satisfy $u(\pi, t) = 0$, we must choose λ such that $\sin(\sqrt{\lambda}\pi) = 0$. As $\sin(x) = 0$ exactly when $x = n\pi,\ \ n = 0, 1, 2, 3, \ldots$, this means that

$$\boxed{\lambda = n^2}\ \ n = 0, 1, 2, 3, \ldots \tag{9.6}$$

To summarize, we now have a whole family of functions which satisfies both the differential equation, and the boundary values, namely

$$u_n(x, t) = e^{-n^2\kappa t}\sin(nx)\ \ n = 1, 2, 3, \ldots$$

and since the problem is homogeneous, any constant multiple of $u_n(x, t)$ is a solution also.

However, we now that the differential equation and boundary condition are homogeneous, so the most general solution is a linear combination of the u_n's.

$$\boxed{u(x, t) = \sum_{n=1}^{\infty} b_n u_n(x, t) = \sum_{n=1}^{\infty} b_n e^{-n^2\kappa t}\sin(nx)} \tag{9.7}$$

This solution functions has an initial value

$$u(x, 0) = \sum_{n=1}^{\infty} a_n u_n(x, 0) = \sum_{n=1}^{\infty} a_n \sin(nx) = f(x). \tag{9.8}$$

Thus we now know how to solve the Dirichlet problem for the homogeneous diffusion equation whenever the initial condition can be written as a sum of functions of the form $\sin(nx)$.

Strictly speaking, we need to formally prove that this series converges, and prove that this can represent any initial value $f(x)$. This is called a *Fourier Sine Series*. The numbers b_n are called the *Fourier Coefficients* of f. This proof is non-trivial, and we will not do it here.

9.4 The solution for general $f(x)$

If the initial condition $f(x)$ is the sum of a finite number of terms of the form $\sin(nx)$ the solution is straightforward.

Example 9.1. Find the solution to

$$\begin{array}{rcl} u_t = \kappa u_{xx} & 0 < x < \pi, t > 0 & \mathbb{DE}: \\ u(0, t) = 0 \quad u(\pi, t) = 0 & t > 0 & \mathbb{BC}: \\ u(x, 0) = 5\sin 3x + 2.7\sin 100x & 0 < x < \pi, & \mathbb{IC}: \end{array}$$

Solution: The solution can be found by inspection; looking at the initial condition (9.12) associated with the general solution(9.7), we see that choosing $b_3 = 5$ and $b_{100} = 2.7$ and setting all the remaining terms to zero yields

$$\boxed{u(x,t) = 5e^{-3^2\kappa t}\sin(3x) + 2.7e^{-100^2\kappa t}\sin(100x).}$$

What about all the other possible initial conditions?

To solve the general problem we will make use of the following fact, the proof of which is left as an exercise:

The orthogonality condition

$$\boxed{\int_0^\pi \sin(nx)\sin(mx)dx = \begin{cases} 0 & n \neq m \\ \frac{\pi}{2} & n = m \end{cases}}$$

To calculate the Fourier coefficients, start with

$$f(x) = \sum_{n=1}^{\infty} b_n \sin(nx).$$

Multiply both sides by $\sin(mx)$ and integrate. We get

$$\begin{aligned} \int_0^\pi f(x)\sin(mx)dx &= \int_0^\pi \sum_{n=1}^{\infty} b_n \sin(nx)\sin(mx)dx \\ &= \sum_{n=1}^{\infty} b_n \int_0^\pi \sin(nx)\sin(mx)dx. \end{aligned}$$

Because of the orthogonality condition, all the terms in the sum are 0 except when $n = m$, in which case we get $\frac{\pi}{2}$. Thus

$$\sum_{n=1}^{\infty} b_n \int_0^\pi \sin(nx)\sin(mx)dx = b_m\frac{\pi}{2} \ !$$

Thus the formula to calculate the Fourier Coefficients is

$$\boxed{b_m = \frac{2}{\pi}\int_0^\pi f(x)\sin(mx)dx} \quad m = 1, 2, 3, \ldots \ .$$

Example 9.2. Find the solution to

$$\begin{array}{rcl} u_t = \kappa u_{xx} & 0 < x < \pi, t > 0 & \mathbb{DE}: \\ u(0,t) = 0 \quad u(\pi,t) = 0 & t > 0 & \mathbb{BC}: \\ u(x,0) = x(\pi - x) & 0 < x < \pi, & \mathbb{IC}: \end{array}$$

Solution: From the solution above, we see that

$$\begin{aligned} b_m &= \frac{2}{\pi}\int_0^\pi f(x)\sin(mx)dx \\ &= \frac{2}{\pi}\int_0^\pi x(\pi - x)\sin(mx)dx \\ &= \begin{cases} 0 & n \quad \text{e}ven \\ \dfrac{8}{\pi n^3} & n \quad \text{o}dd \end{cases} \end{aligned}$$

So the full solution is

$$\boxed{u(x,t) = \frac{8}{\pi}\sum_{n=1,3,5,\cdots}^{\infty} \frac{e^{-n^2\kappa t}}{n^3}\sin(nx)} \tag{9.9}$$

9.5 THE NEUMANN PROBLEM

If instead of specifying the temperature at the endpoints, we specify the heat flux we obtain the Neumann problem:

The Neumann Problem for the Diffusion Equation
(Homogeneous Boundary Conditions)

$$\begin{array}{rlcl} & u_t = \kappa u_{xx} & 0 < x < \pi, t > 0 & \mathbb{DE}: \\ u_x(0,t) = 0 & u_x(\pi,t) = 0 & t > 0 & \mathbb{BC}: \\ & u(x,0) = f(x) & 0 < x < \pi, & \mathbb{IC}: \end{array}$$

The boundary conditions can be interpreted physically as saying the endpoints are insulated; basically there is no heat flux out of the ends or the bar.

We wish the solutions (9.5) we found for $u(x,t)$ to satisfy the homogeneous boundary conditions $u_x(0,t) = u_x(\pi,t) = 0$. Note that when $\lambda = 0$ we found that

$$u(x,t) = C(Ax + B) \Rightarrow u_x(x,t) = CA,$$

and

$$u_x(0,t) = AC = 0, \qquad u_x(\pi,t) = AC = 0,$$

from which we deduce $AC = 0$ but we have a solution

$$u(x,t) = u_0(x,t) = 1,$$

or any multiple of this solution.

In the case where

$$u(x,t) = Ce^{-\lambda\kappa t}\left(A\cos(\sqrt{\lambda}x) + B\sin(\sqrt{\lambda}x)\right),$$

we find that

$$u_x(x,t) = Ce^{-\lambda\kappa t}\left(-A\sqrt{\lambda}\sin(\sqrt{\lambda}x) + B\sqrt{\lambda}\cos(\sqrt{\lambda}x)\right),$$

and

$$u_x(x,0) = CB\sqrt{\lambda} = 0,$$

From which we deduce $CB = 0$. At $x = \pi$ we now find

$$u_x(x,\pi) = -AC\sqrt{\lambda}\sin(\sqrt{\lambda}\pi),$$

To satisfy this condition we must choose λ such that $\sin(\sqrt{\lambda}\pi) = 0$. As $\sin(x) = 0$ exactly when $x = n\pi,\ n = 0, 1, 2, 3, ...$, this means that once again

$$\boxed{\lambda = n^2} \quad n = 0, 1, 2, 3, ... \tag{9.10}$$

which yields a whole family of functions which satisfies both the differential equation, and the boundary values, namely

$$u_n(x,t) = e^{-n^2\kappa t}\cos(nx) \quad n = 1, 2, 3, ...$$

and since the problem is homogeneous, any constant multiple of $u_n(x,t)$ is a solution also. However, we now that the differential equation and boundary condition are homogeneous, so the most general solution is a linear combination of the u_n's.

$$\boxed{u(x,t) = \sum_{n=0}^{\infty} a_n u_n(x,t) = a_0 + \sum_{n=1}^{\infty} a_n e^{-n^2\kappa t}\cos(nx)} \tag{9.11}$$

This solution functions has an initial value

$$u(x,0) = a_0 + \sum_{n=1}^{\infty} a_n u_n(x,0) = a_0 + \sum_{n=1}^{\infty} a_n \cos(nx) = f(x). \tag{9.12}$$

Thus we now know how to solve the Dirichlet problem for the homogeneous diffusion equation whenever the initial condition can be written as a sum of functions of the form $\cos(nx)$.

Strictly speaking, we need to formally prove that this series converges, and prove that this can represent any initial value $f(x)$. This is called a *Fourier Cosine Series*. The numbers b_n are called the *Fourier Coefficients* of f. This proof is non-trivial, and we will not do it here.

To solve the problem we again make use of an orthogonality condition, *The orthogonality condition*

$$\boxed{\int_0^{\pi}\cos(nx)\cos(mx)dx = \begin{cases} 0 & n \neq m \\ \frac{\pi}{2} & n = m = 1, 2, 3, \ldots \\ 1 & n = m = 0 \end{cases}}$$

To calculate the Fourier coefficients, start with

$$f(x) = \sum_{n=1}^{\infty} a_n \sin(nx).$$

Multiply both sides by $\cos(mx)$ and integrate. We get

$$\begin{aligned} \int_0^{\pi} f(x)\cos(mx)dx &= \int_0^{\pi} \sum_{n=1}^{\infty} a_n \cos(nx)\cos(mx)dx \\ &= \sum_{n=1}^{\infty} a_n \int_0^{\pi} \cos(nx)\cos(mx)dx. \end{aligned}$$

Because of the orthogonality condition, all the terms in the sum are 0 except when $n = m$, from which we deduce the formula to calculate the Fourier Coefficients is

$$\boxed{a_0 = \frac{1}{\pi}\int_0^{\pi} f(x)\,dx \qquad a_m = \frac{2}{\pi}\int_0^{\pi} f(x)\cos(mx)dx \;\; m = 1, 2, 3, \ldots.}$$

Example 9.3. Find the solution to

$$\begin{array}{rcc} u_t = \kappa u_{xx} & 0 < x < \pi, t > 0 & \mathbb{DE}: \\ u_x(0,t) = 0 \quad u_x(\pi,t) = 0 & t > 0 & \mathbb{BC}: \\ u(x,0) = x & 0 < x < \pi, & \mathbb{IC}: \end{array}$$

Solution: From the solution above, we see that

$$a_0 = \frac{1}{\pi}\int_0^{\pi} f(x)\,dx = \frac{1}{\pi}\int_0^{\pi} x\,dx = \frac{1}{2}$$

and

$$\begin{aligned} a_m &= \frac{2}{\pi}\int_0^{\pi} f(x)\cos(mx)dx \\ &= \frac{2}{\pi}\int_0^{\pi} x\cos(mx)dx \\ &= \begin{cases} 0 & n \quad \text{e}ven \\ -\dfrac{4}{\pi n^2} & n \quad \text{o}dd \end{cases} \end{aligned}$$

So the full solution is

$$\boxed{u(x,t) = \frac{1}{2} - \frac{4}{\pi}\sum_{n=1,3,5,\cdots}^{\infty} \frac{e^{-n^2\kappa t}}{n^2}\cos(nx)} \tag{9.13}$$

9.5.1 Sturm-Liouville Eigenvalue Problems

In this section, we will consider the general eigenvalue problem as

$$\mathcal{L}y = \lambda y, \quad a < x < b \qquad y(a) = 0, \quad y(b) = 0,$$

where $\mathcal{L}y = -y''$. We introduce the L^2 inner-product

$$\langle u, v \rangle = \int_a^b uv \, dx.$$

We can show the differential operator $\mathcal{L}$ is self-adjoint via integration by parts,

$$\begin{aligned} \langle u, \mathcal{L}v \rangle &= -\int_a^b uv'' \, dx \\ &= \int_a^b u'v' \, dx - uv'|_{x=a}^{x=b} \\ &= -\int_a^b u''v' \, dx + u'v - uv'|_{x=a}^{x=b}. \end{aligned}$$

Now if u and v satisfy the DE's boundary conditions, that is $u(a) = v(a) = 0$ and $u(b) = v(b) = 0$, we can deduce the operator is self-adjoint,

$$\langle u, \mathcal{L}v \rangle = \langle \mathcal{L}u, v \rangle.$$

To show the eigenvalues are real, assume that y_n is an eigenvalue associated with λ_n. Then, since $\mathcal{L}$ is a real operator, we know that $\bar{y}_n$ and $\bar{\lambda}_n$ also satisfy the eigenvalue problem (here bars denote complex conjugates). That is

$$-(y_n)'' = \lambda_n y_n \qquad \Rightarrow \qquad -(\bar{y}_n)'' = \bar{\lambda}_n \bar{y}_n$$

Now from the self-adjointness of the operator

$$\lambda_n \langle \bar{y}_n, y_n \rangle = \langle \bar{y}_n, \mathcal{L}y_n \rangle = \langle \mathcal{L}\bar{y}_n, y_n \rangle = \bar{\lambda}_n \langle \bar{y}_n, y_n \rangle$$

or rearranging

$$(\lambda_n - \bar{\lambda}_n) \langle \bar{y}_n, y_n \rangle = (\lambda_n - \bar{\lambda}_n) \int_a^b \bar{y}_n y_n \, dx = (\lambda_n - \bar{\lambda}_n) \int_a^b |y_n|^2 \, dx = 0.$$

From which we deduce that either $\lambda_n = \bar{\lambda}_n$ or $y_n = 0$ identically for $a < x < b$ (assuming continuity). Consequently λ_n is real. Moreover, since the

DE has real coefficients, we can now conclude that there is a real-valued solution for y_n also.

To show that λ_n is positive, note that

$$\lambda_n \langle y_n, y_n \rangle = \langle y_n, \mathcal{L} y_n \rangle = -\int_a^b y_n (y_n)'' \, dx = \int_a^b |(y_n)'|^2 \, dx,$$

where we have used the fact that the boundary terms vanish when integrating by parts. More succinctly, we can write

$$\lambda_n = \frac{||(y_n)'||^2}{||(y_n)||^2} \, .$$

Clearly, the right-hand side is non-negative. Moreover, $\lambda_n = 0$ is only possible if $(y_n)' = 0$ for $a < x < b$, that is if y_n is constant. But $y_n(a) = 0$, so if y_n is constant it must vanish identically on the interval. Consequently, we conclude the eigenvalues are positive.

Finally, we wish to show that if we have two eigenfunctions y_n and y_m with distinct associated eigenvalues $\lambda_n \neq \lambda_m$ that the eigenfunctions are orthogonal, that is $\langle y_m, y_n \rangle = 0$. Note

$$\lambda_n \langle y_m, y_n \rangle = \langle y_m, \mathcal{L} y_n \rangle = \langle \mathcal{L} y_m, y_n \rangle = \lambda_m \langle y_m, y_n \rangle$$

or rearranging

$$(\lambda_n - \lambda_m) \langle y_m, y_n \rangle = 0.$$

As $\lambda_n \neq \lambda_m$ we conclude $\langle y_m, y_n \rangle = 0$, that is that the eigenfunctions are orthogonal.

Note that if we choose $a = 0$ and $b = \pi$ we find

$$\lambda_n = n^2 \qquad y_n = \sin(nx) \qquad for \quad n = 1, 2, 3, \cdots$$

The orthogonality conditions used to solve the Dirichlet problem now follow from the fact that the $\{y_n\}$ are eigenfunctions associated with different eigenvalues for this Sturm-Liouville problem.

9.6 Challenge Problems for Lecture 5

Problem 9.1. Use Maple to graph the solution to the homogeneous Dirichlet problem for the diffusion equation with initial condition $f(x) = (\sin(x))^2$ on $[0, \pi]$.

Problem 9.2. Rework the solution to the homogeneous Dirichlet problem for a bar of length L instead of length π. That is, solve

$$\begin{array}{rcll} & U_t = \kappa U_{xx} & 0 < x < L, t > 0 & \mathbb{DE}: \\ U(0,t) = 0 & U(L,t) = 0 & t > 0 & \mathbb{BC}: \\ & U(x,0) = f(x) & 0 < x < L. & \mathbb{IC}: \end{array}$$

Problem 9.3. Solve the Neumann problem :

$$\begin{array}{rcll} & u_t = \kappa u_{xx} & 0 < x < \pi, t > 0 & \mathbb{DE}: \\ u_x(0,t) = 0 & u_x(\pi,t) = 0 & t > 0 & \mathbb{BC}: \\ & u(x,0) = f(x) & 0 < x < \pi, & \mathbb{IC}: \end{array}$$

For $f(x) = 2 + 3\cos(2x)$ using separation of variables. Plot the solution in Maple. What happens as $t \to \infty$?

Problem 9.4. Solve the Dirichlet problem when the boundary conditions are not homogeneous. That is, solve it for

$$\begin{array}{rcll} & U_t = \kappa U_{xx} & 0 < x < L, t > 0 & \mathbb{DE}: \\ U(0,t) = a & U(L,t) = b & t > 0 & \mathbb{BC}: \\ & U(x,0) = f(x) & 0 < x < L. & \mathbb{IC}: \end{array}$$

Hint: First find a simple solution $g(x)$ which satisfies the DE and the BC.