Section 4.2: Separating Variables in the Parabolic Equation

The technique for separating variables is applied to the parabolic partial differential equation (PDE). Recall that the heat and diffusion equations are parabolic.

Consider the following boundary value problem for heat flow. Define the function u(x,t) to be the temperature in the block shown in Figure 4.2.1. Assume the ends of the block at x=0,L are insulated so that heat cannot flow through the boundaries there. The boundary conditions for insulated boundaries can be written using the results from Section 1.8. The thermal flux is defined as the thermal energy flowing across a unit surface area in a unit time (power/area)

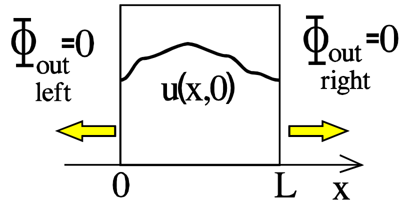

Figure 4.2.1: u(x,0) is the initial temperature distribution. The right-hand and left-hand boundaries are insulating so that the heat flux Φ throught the sides must be zero for all time.

$$\vec{\Phi} = -K\nabla u$$

Applying this definition of flux to the boundaries provides

$$0 = \Phi_{\substack{out\\right}} = \hat{x}\cdot\left(-K\nabla u\right)\Big|_L = -Ku_x(L,t)$$

$$0 = \Phi_{\substack{out\\left}} = \left(-\hat{x}\right)\cdot\left(-K\nabla u\right)\Big|_0 = Ku_x(0,t)$$

The boundary value problem is then written as

$$\begin{array}{lll} \text{PDE:} & u_t - ku_{xx} = 0 & x \in (0,L) \\ \text{BC1:} & u_x(0,t) = 0 & \\ \text{BC2:} & u_x(L,t) = 0 & \\ \text{IC1:} & u(x,0) = f(x) & \end{array}$$

As mentioned in the introduction to Chapter 3, there are several steps for solving the boundary value problem with homogeneous boundary conditions and homogeneous partial differential equation. Notice that "x" takes on values in $x \in (0,L)$. As discussed in Chapter 3, the domain determines the normalization constant for the basis vectors.

Topic 4.2.1: Step 1: Separate Variables

This first step consists of separating variables using $u(x,t) = X(x)T(t)$ so that the PDE

$$u_t(x,t) = ku_{xx}(x,t)$$

becomes

$$X(x)T'(t) = kX''(x)T(t)$$

where the primes indicate derivatives. Dividing by XT and keeping "k" with T (this is always the case), provides

$$\frac{X''}{X} = \frac{T'}{kT} \tag{4.2.1}$$

The boundary conditions for u(x,t) involves x and they are necessary for the Sturm-Liouville problem that gives the basis vectors. To keep the Sturm-Liouville equation as simple as possible, it is traditional to keep "k" with T.

The ratio X''/X involves only "x". Normally changing the value of x should change the ratio X''/X. But this ratio cannot change because the right-hand ratio $T'/(kT)$ cannot change since it does not depend on x. This argument suggests that the two ratios in Equation 4.2.1 must be equal to a constant, say $-\lambda$ (also turn out to the eigenvalues in the Sturm-Liouville problem).

$$\frac{X''(x)}{X(x)} = -\lambda = \frac{T'(t)}{kT(t)} \tag{4.2.2}$$

The constant $-\lambda$ is the "separation constant".

Writing u(x,t) as the product XT also affects the boundary conditions. The first boundary condition BC1

$$u_x(0,t) = 0$$

becomes

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

Assume the function T(t) is not identically zero, the boundary condition at x=0 is therefore

$$X'(0) = 0$$

If the original boundary condition had not been homogeneous, there could not have been any conclusion on the boundary condition for X'. For example if $u_x(0,t) = 10$ then $X'(0) = 10/T(t)$ but T(t) is not known. The second boundary condition BC2 becomes

$$X'(L) = 0$$

The original boundary value problem is now stated as

ODE1: $X''(x) + \lambda X(x) = 0$ ODE2: $T'(t) + \lambda k T(t) = 0$

BC3: $X'(0) = 0$

BC4: $X'(L) = 0$

Notice that the initial condition $u(x,0) = f(x)$ cannot be separated since it is not homogeneous. This means that there is no initial condition to accompany ODE2 for T. The solution still requires the sum over products $X_\lambda(x)T_\lambda(t)$; the initial condition IC1 is then applied to the summation.

Topic 4.2.2: Step 2: Solve a Sturm-Liouville Problem

Solve a Sturm-Liouville problem of the form

$$\hat{O}X_\lambda = -\lambda X_\lambda \qquad \text{plus BCs on X}$$

for all possible eigenfunctions X_λ and eigenvalues $-\lambda$. Each different eigenvalue can yield a different eigenfunction and so the eigenfunctions X_λ are labeled by the eigenvalues.

For the case above, the boundary conditions on X identify the Sturm-Liouville Problem as

ODE1: $X''(x) + \lambda X(x) = 0$

BC3: $X'(0) = 0$

$$\text{BC4:} \qquad X'(L) = 0$$

The second order equation has a general solution that depends on the sign of λ; this is readily verified by substituting e^{mx} to find $m = \pm\sqrt{-\lambda}$. There are three separate domains of λ. If $\lambda > 0$ then the solutions are oscillatory. If $\lambda = 0$ the solutions are polynomials in x. The case $\lambda < 0$ gives exponentially increasing or decreasing solutions. The technique is outlined in Section A3.3 in Appendix 3.

Case 1: $\lambda < 0$

Define $\lambda = -\alpha^2$ with $\alpha > 0$ (the combination of the negative sign and the square ensures that λ is negative). The Sturm-Liouville problem has the form

$$X''(x) - \alpha^2 X(x) = 0$$
$$X'(0) = X'(L) = 0$$

The general solution X(x) has the form

$$X(x) = c_1 e^{\alpha x} + c_2 e^{-\alpha x} \qquad \text{with } \alpha > 0$$

In principle, X can be indexed by α, but that won't be necessary in this case. Now apply the first boundary condition of $X'(0) = 0$ to get

$$0 = X'(0) = \alpha c_1 e^{\alpha 0} - \alpha c_2 e^{-\alpha 0} = \alpha\left(c_1 - c_2\right)$$

Using $\alpha \neq 0$ (since $\alpha > 0$) provides $c_1 = c_2$. The solution X now has the form

$$X(x) = c_1\left[e^{\alpha x} + e^{-\alpha x}\right]$$

Next, apply the second BC of $X'(L) = 0$ to find

$$0 = X(L) = c_1\left[e^{\alpha L} + e^{-\alpha L}\right]$$

Neither α nor L is zero so that c_1=0 and therefore c_2=0. The only solution for this case is X=0 which is the trivial solution...it is not acceptable.

Case 2: $\lambda = 0$

The differential equation ODE1 becomes

$$\text{ODE1:} \qquad X''(x) = 0$$
$$\text{BC3:} \qquad X'(0) = 0$$
$$\text{BC4:} \qquad X'(L) = 0$$

The general solution to ODE1 is found by integrating twice

$$X(x) = c_0 + c_1 x$$

Boundary condition BC3 yields $0 = c_1$. Using $X(x) = c_0$, boundary condtion BC4 does not provide any information on c_0 . The present case gives the first basis vector n=0 corresponding to the eigenvalue $\lambda = 0$ as $X_0(x) = c_0$. Require the "length" of X_0 to be unity

$$1 = \left\|X_0\right\|^2 = \left\langle X_0 \middle| X_0 \right\rangle = \int_0^L dx\ \left|c_0\right|^2 \quad \to \quad c_0 = \frac{1}{\sqrt{L}}$$

where an arbitrary phase is ignored. Sometimes books set c_0=1 without caring about normalizing the vectors. However, taking the inner products at the end of the problem become more tedious. The first basis function is

$$X_0(x) = \frac{1}{\sqrt{L}} \qquad \lambda_0 = \alpha_0^2 = 0 \tag{4.2.3}$$

Case 3: $\lambda > 0$

It is customary to set $\lambda = \alpha^2$ with $\alpha > 0$ for this case. The Liouville problem has the form

ODE1:	$X'' + \alpha^2 X = 0$
BC3:	$X'(0) = 0$
BC4:	$X'(L) = 0$

The general solution to the ordinary differential equation ODE1 is

$$X(x) = c_1 \cos(\alpha x) + c_2 \sin(\alpha x)$$

Apply the boundary condition BC3 to find

$$0 = X(0) = -\alpha c_1 \sin(\alpha 0) + \alpha c_2 \cos(\alpha 0)$$

and therefore $c_2 = 0$ since $\alpha \neq 0$. The solution so far is

$$X(x) = c_1 \cos(\alpha x) \tag{4.2.4}$$

Next, apply boundary condition BC4 to find

$$0 = X'(L) = \alpha c_1 \sin(\alpha x)$$

We know that α is not zero and we don't want $c_1 = 0$ since then X(x) is just the trivial solution. Therefore, require the sine function to be zero which occurs for

$$\alpha = \frac{n\pi}{L} \qquad \text{where n=1,2,3...} \tag{4.2.5}$$

Notice that n=0 is not allowed since the starting assumption required $\alpha \neq 0$ and besides, α=0 gives Case 2. Also notice that negative values of "n" are not included because sine is an odd function and negative "n" only trivially changes the sign of c_1.

Notice that α depends on "n" and hence so does X(x). The solution should be suscripted with n (or equivalently with the eigenvalue λ)

$$X_n(x) = c_n \cos\left(\frac{n\pi x}{L}\right) \tag{4.2.6}$$

where the coefficient c_1 is subscripted with "n" just in case it depends on "n". Notice that the boundary conditions picked the cosines rather than the sines as the basis functions. The eigenvalue $-\lambda$ is evident by comparing ODE1 with the eigenfunction equation

$$\hat{O} X_\lambda = -\lambda X_\lambda \qquad \text{where} \qquad \hat{O} = d^2/dx^2$$

to find $\lambda = \alpha^2$. Therefore the eigenvalues $-\lambda$ are found

$$\lambda = \alpha^2 = \left(\frac{n\pi}{L}\right)^2 \rightarrow \quad -\lambda = -\left(\frac{n\pi}{L}\right)^2 \qquad n = 0, 1, 2, \ldots$$

Notice that the case n=0 is included because of Case #2.

Normalizing the eigenfunction X_n on the interval (0,L) determines the coefficients c_n

$$1=\|X_n\|^2=\langle X_n\,|\,X_n\rangle=\frac{L}{2}|c_n|^2 \quad \rightarrow \quad c_n=\sqrt{\frac{2}{L}}$$

where the last step ignores an arbitrary phase.

Taken together, the eigenfunctions for Cases 2 and 3 corresponding to all of the eigenvalues gives a complete basis set for the solution space

$$B_c=\left\{\frac{1}{\sqrt{L}},\sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right): x\in(0,L) \text{ and n=1,2,...}\right\}$$

Notice that allowing n=0 or n<0 does not generate any new basis functions.

The reader is familiar with the cosine basis set B_c from the discussion in the previous chapter covering the Cosine series orthonormal expansion (Topic 3.8.1). It is very important to realize that the normalization constants depend not only on the size of the interval [0,L] but also on the fact that $\alpha_n = n\pi/L$. To see this, suppose to the contrary that for some reason $\alpha_n \neq n\pi/L$ even though the interval is [0,L] (we will see an example of this in later chapters when we discuss the composition of two functions). The normalization constant for

$$\phi_\alpha(x)=c_\alpha\cos(\alpha x)$$

is found from the normalization condition (assume c_α is real)

$$1=\|\phi_\alpha\|^2=c_\alpha{}^2\langle\cos(\alpha x)|\cos(\alpha x)\rangle=\frac{c_\alpha^2}{2}\left[L+\frac{\sin(2\alpha x)}{2\alpha}\right]$$

The normalization constant is

$$c_\alpha=\left[\frac{4\alpha}{2\alpha L+\sin(2\alpha L)}\right]^{1/2}$$

Topic 4.2.3: Step 3: Find T(t)

The differential equation for T(t) comes from the separation of variables (ODE2 in Step 1)

$$T'(t)+\lambda k\,T(t)=0 \tag{4.2.7}$$

where k, which is related to a diffusion coefficient for the parabolic equation, is known from the initial partial differential equation. Equation 2.2.7 is NOT a sturm-Liouville equation since the allowed separation constants are already known from Step 2; the eigenfunctions $X_n(x)$ are also known. At this point, Equation 2.2.7 must be solved as an ordinary differential equation with the constants λ,k assumed known. Notice that the initial condition u(x,0)=f(x) does not provide a boundary condition since it does not give useful information for T(0). The general solution to Equation 4.2.7 is easily determined to be

$$T(t)=c_1 e^{-\lambda kt}$$

The function T should be indexed with a λ or an "n" because of the λ on the right-hand side. The arbitrary constant c_1 can be set to c_1=1 by including an undetermined constant in the sum over basis vectors. Note that $\lambda=0$ should be handled separately; however, $T'=0 \Rightarrow T=c_0$ agrees with $T_n=c_n e^{-\lambda_n kt}$ for this problem.

Topic 4.2.4: Step 4: The general Solution u(x,t)

The product $u_n(x,t) = X_n T_n$ for each n=0,1,2,... is a solution of the orginal partial differential equation. The full general solution becomes a sum over the basis set of eigenvectors using an index to represent the allowed eigenvalues

$$u(x,t) = \sum_{n=0}^{\infty} \beta_n u_n(x,t) = \sum_{n=0}^{\infty} \beta_n X_n(x) T_n(t) \qquad (4.2.8)$$

Many times, especially for perturbation theory or the method of eigenfunction expansions, β_n is viewed as time dependent and written as

$$\beta_n(t) = \beta_n T_n(t)$$

The general solution then has the form

$$u(x,t) = \sum_{n=0}^{\infty} \beta_n(t) X_n(x)$$

or as

$$|u(t)\rangle = \sum_{n=0}^{\infty} \beta_n(t) |X_n\rangle$$

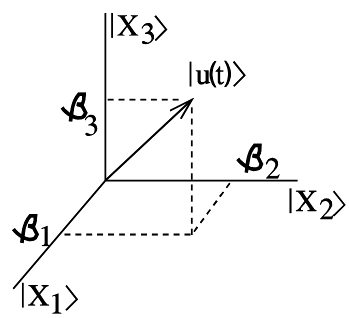

Figure 4.2.1: The vector representation of the solution $u(x,t) = \langle x | u(t) \rangle$.

where $|X_n\rangle = |n\rangle$ are basis vectors in an infinite dimensional Hilbert space. We will explicitly show the "t" in $\beta_n(t)$ when $\beta_n(t) = \beta_n T_n(t)$. When β is viewed as a constant, we will write β (without the "t") or explicitly as $\beta = \beta(0)$.

Of course the basis functions and eigenvalues can be substituted into Equation 4.2.8 to obtain

$$u(x,t) = \frac{\beta_0}{\sqrt{L}} e^{-0kt} + \sum_{n=1}^{\infty} \beta_n \left(\sqrt{\frac{2}{L}} \cos \frac{n\pi x}{L} \right) \exp\left[-\left(\frac{n\pi}{L} \right)^2 kt \right]$$

or

$$u(x,t) = \frac{\beta_0}{\sqrt{L}} + \sum_{n=1}^{\infty} \beta_n \left(\sqrt{\frac{2}{L}} \cos \frac{n\pi x}{L} \right) \exp\left[-\left(\frac{n\pi}{L} \right)^2 kt \right]$$

Notice that the components of the vector $|u(t)\rangle$ in Figure 4.2.1 for this case are (for n>0)

$$\beta_n(t) = \beta_n(0) \exp\left[-\left(\frac{n\pi}{L} \right)^2 kt \right]$$

Therefore, the length of the vector $|u(t)\rangle$ and the components of $|u(t)\rangle$ (except for n=0) *decrease* with time. In fact, because the time constants $\tau_n = (n\pi / L)^{-2}$ are all different from each other, the vector $|u(t)\rangle$ *rotates* as it *shrinks*! For very large times, the solution approaches $\beta_0 / \sqrt{L}$. The picture in Hilbert space helps to visualize the behavior of the solution. For more information refer to Topic 4.2.6.

Topic 4.2.5: Step 5: Apply the Initial Condition

The initial condition is u(x,0)=f(x) which requires

$$f(x) = u(x,0) = \frac{\beta_0}{\sqrt{L}} + \sum_{n=1}^{\infty} \beta_n \left(\sqrt{\frac{2}{L}} \cos \frac{n\pi x}{L} \right) = \sum_{n=0}^{\infty} \beta_n \left| X_n \right\rangle \qquad (4.2.9)$$

where the function f(x) is assumed to be known from the initial statement of the boundary value problem. Summations like that in Equation 4.2.9 are discussed in Chapter 3. The coefficients β_n are found by projecting the known function f(x) onto each basis vector

$$\beta_0 = \left\langle X_0 \middle| f \right\rangle = \left\langle \frac{1}{\sqrt{L}} \middle| f \right\rangle = \frac{1}{\sqrt{L}} \int_0^L dx\, f(x) \qquad \text{and}$$

$$\beta_n = \left\langle X_n \middle| f \right\rangle = \left\langle \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L} \right) \middle| f(x) \right\rangle = \int_0^L dx\, \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L} \right) f(x) \qquad \text{for } n \geq 1$$

Notice that β_0 is related to an average over f(x).

Example 4.2.1: What are the β_n for the heat equation if

$$u(x,0) = f(x) = \cos\left(\frac{2\pi x}{L} \right)$$

This is really easy by recognizing that the function f(x) can be written as a basis vector

$$f(x) = \sqrt{\frac{L}{2}} \left[\sqrt{\frac{2}{L}} \cos\left(\frac{2\pi x}{L} \right) \right] = \sqrt{\frac{L}{2}}\, X_2$$

Then for $n \neq 2$

$$\beta_n = \left\langle X_n \middle| f \right\rangle = \sqrt{\frac{L}{2}} \left\langle X_n \middle| X_2 \right\rangle = 0$$

while for n=2

$$\beta_2 = \left\langle X_2 \middle| f \right\rangle = \sqrt{\frac{L}{2}} \left\langle X_2 \middle| X_2 \right\rangle = \sqrt{\frac{L}{2}}$$

Of course, all of the components β_n are obtained because the set $\left\{ \left| X_n \right\rangle = \left| n \right\rangle \right\}$ is a basis set with the orthonormality relation

$$\left\langle X_n \middle| X_m \right\rangle = \delta_{nm}$$

Topic 4.2.6: The Behavior of the Solution for Large Times

For the heat problem, the length of the solution vector $\|u\|$ can be found from the inner product (with β_n assumed to be real) as

$$\|u(t)\|^2 = \langle u(t)|u(t)\rangle = \left[\sum_{n=0}^{\infty} \beta_n^*(t)\langle n|\right]\left[\sum_{m=0}^{\infty} \beta_m(t)|m\rangle\right]$$
$$= \sum_{m,n=0}^{\infty} \beta_n(t)\beta_m(t)\delta_{mn} = \sum_{n=0}^{\infty} \beta_n^2(t) \qquad (4.2.10)$$

where

$$\beta_0(t) = \beta_0 \qquad\qquad \beta_n(t) = \beta_n \exp\left[-k\left(\frac{n\pi}{L}\right)^2 t\right] \qquad (4.2.11)$$

and β_n are independent of time. Equation 4.2.10 is a generalized Pythagorean's theorem. The length of u(x,t) is found from

$$\|u(t)\|^2 = \sum_{n=0}^{\infty} \beta_n^2(t) = \beta_0^2 + \sum_{n=1}^{\infty} \beta_n^2 e^{-2k\left(\frac{n\pi}{L}\right)^2 t} \qquad (4.2.11)$$

The length of the vector $|u(t)\rangle$ is seen to change with time and it approaches β_0 as $t \to \infty$

$$\|u(t)\| \to \beta_0 \qquad (4.2.12)$$

As time increases, the temperature u(x,t) at every point x approaches an average value as can be seen from Equation 4.2.12 as follows.

$$\beta_0 = \left\langle \frac{1}{\sqrt{L}} \middle| u(x,0) \right\rangle = \frac{1}{\sqrt{L}} \int_0^L dx\ u(x,0) = \sqrt{L}\,\langle u(x,0)\rangle \qquad (4.2.13)$$

where the average $\langle u(x,0)\rangle$ is defined to be

$$\langle u(x,0)\rangle \equiv \frac{1}{L}\int_0^L dx\ u(x,0)$$

from elementary calculus. Therefore, Equation 4.2.13 shows that the first term in the Fourier expansion for the solution

$$\frac{\beta_0}{\sqrt{L}} = \langle u(x,0)\rangle$$

is just the average of the initial temperature distribution. That is, the solution u(x,t) approaches the average of the initial temperature distribution as time increases. The discussion in this section shows that this behavior is typical of all parabolic equations. Figure 4.2.2 shows the behavior for an initial Gaussian distribution. If L is very large then the width of the curve increases but the displacement above the x-axis is small. The motion might typify a cloud of smoke as it diffuses with time.

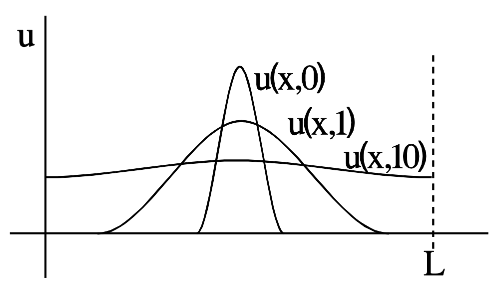

Figure 4.2.2: An initial Gaussian distribution spreads with time and approaches the average of the initial distribution.

Notice $\|u(t)\| \to \beta_0 = \sqrt{L}\langle u(x,0)\rangle$ is due to the insulating boundaries. The function "u" is similar to temperature which is an expression of the energy. The total energy of the system must be constant because of the insulating boundaries. This means that the energy redistributes itself but does not change the average. For *non-insulating* boundaries, say u(0,t)=0=u(L,t), we have $\beta_0 = 0$ which implies the temperature decays to zero.

Topic 4.2.7: A Note on the Complex Basis Functions

The values $\lambda < 0$ were not allowed for the Sine or Cosine basis set. However, replacing Sines and Cosines with the basis set

$$\left\{ X_n = \frac{e^{ik_n x}}{\sqrt{2L}} \right\}$$

with the expansion

$$u = \sum_n \beta_n(t) X_n(x)$$

requires the negative k to be included. This occurs because the sines and cosines are condensed into the single complex exponential. Refer to the end of the next section.