18.03 The Heat Equation

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1 Introduction

The goal in this note is to derive the heat equation from Newton's law of cooling. We can get most of the way using just mathematics. The final piece of the puzzle requires the use of an empirical principle of heat flow.

In outline: First we'll set up the problem of heat flow in a bar. Then will discretize the problem and analyze $n \times n$ systems of equations based on Newton's law of cooling. Finally, we'll let the discrete stepsize go to 0 to get the continuous heat equation as the limit of the discretized system.

2 Notation

We have a small notational conflict to resolve. In discrete systems, we usually represent components of vectors with subscripts, e.g., $\mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}$. While for continuous systems, we use function notation, e.g., $u(x,t)$. Since we are going to take the limit of a discrete system to get a continuous one, we need to make some notational choices. For eigenvectors of our discrete system, we'll use functional notation with square brackets, e.g.,

$$\mathbf{v} = \begin{bmatrix} \mathbf{v}[1] \\ \mathbf{v}[2] \\ \mathbf{v}[3] \end{bmatrix}.$$

For the functions giving the temperature in pieces of our discrete system, we'll use subscripts, e.g.

$$\mathbf{u}(t) = \begin{bmatrix} u_1(t) \\ u_2(t) \\ u_3(t) \end{bmatrix}.$$

It's not a perfect notational system, but it will suffice for our purposes

3 Continuous heat equation

Suppose we have a heated bar where the temperature varies both in time and in position along the bar. To be specific, we assume we have a rod of length L, which is thin enough that the temperature doesn't vary in the vertical direction. So we can describe the temperature of the bar by a function of two variables $u(x,t)$, which gives the temperature at time t at position x.

We will assume that the sides of the bar are insulated, so that no heat passes through them. We will also assume that the ends of the bar are kept in an ice bath at $0°$. This is illustrated in the figure below.

Heated rod with temperature varying by position and time: $u(x, t)$.

In ES.1803, we have seen that this is modeled by the heat equation with boundary conditions:

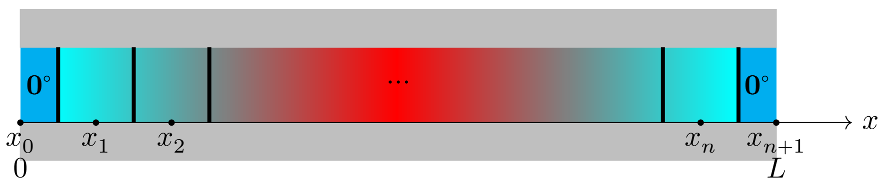
$$\text{PDE}: \; u_t(x,t) = k_0 u_{xx}(x,t) \tag{1}$$
$$\text{BC}: \; u(0,t) = 0, \; u(L,t) = 0. \tag{2}$$

We have also seen that this has modal solutions:

$$u_m(x,t) = \sin\left(\frac{m\pi x}{L}\right) e^{-(m\pi/L)^2 k_0 t}. \tag{3}$$

4 Discrete heat equation

As in previous examples in the course, let's divide the rod into sections and assume the temperature is uniform in each section.



Heated rod divided into pieces.

Let's call the temperature in the jth section $u_j(t)$. Newton's law of cooling gives

$$u_j'(t) \;=\; -k(u_j - u_{j-1}) - k(u_j - u_{j+1}) \;=\; ku_{j-1} - 2ku_j + ku_{j+1} \tag{4}$$

Taking into account the ice baths, we get a system of differential equations. (We show the coefficient matrix for $n = 4$. It follows the same pattern for other values of n.)

$$\mathbf{u}'(t) = A\mathbf{u}, \quad \text{where} \quad \mathbf{u}(t) = \begin{bmatrix} u_1(t) \\ u_2(t) \\ \vdots \\ u_n(t) \end{bmatrix}, \quad \text{and (for } n = 4\text{)} \quad A = \begin{bmatrix} -2k & k & 0 & 0 \\ k & -2k & k & 0 \\ 0 & k & -2k & k \\ 0 & 0 & k & -2k \end{bmatrix}$$

We'll call this equation the discrete heat equation because we've divided the bar into discrete chunks.

For future reference, note the way we divided the bar into sections: The n middle pieces all have width $\Delta x = L/(n+1)$ and centers $x_j = j\Delta x$ and the two end pieces (in the ice baths) are each half that width.

4.1 Eigenvalues and eigenvectors of the matrix A

We know that to solve the discrete heat equation, we must find eigenvalues and eigenvectors of the coefficient matrix A. These are given by

Theorem: Let
$$\theta_m = \frac{m\pi}{n+1} \quad \text{and} \quad \lambda_m = -2k + 2k\cos(\theta_m).$$
For each $m = 1, 2, \ldots, n$, A has eigenvalues λ_m, and corresponding eigenvectors
$$\mathbf{v_m} = \begin{bmatrix} \sin(\theta_m) \\ \sin(2\theta_m) \\ \vdots \\ \sin(n\theta_m) \end{bmatrix}$$

Proof number 1: This can be checked directly using the trigonometric identity
$$\sin((k-1)\theta) + \sin((k+1)\theta) = 2\cos(\theta)\sin(k\theta)$$

The exact value of θ_m only comes into play for the nth entry in the eigenvector. For that entry, the eigenequation takes the form
$$\sin((n-1)\theta_m) - 2\sin(n\theta_m) = (-2 + 2\cos(\theta_m))\sin(n\theta_m)$$

This follows from the previous trig identity with $k = n$ because, for this particular θ_m, we have $\sin((n+1)\theta_m) = 0$.

This proof doesn't give much insight into how we might discover these eigenpairs. The entire next section will be devoted to that.

4.2 Proof number 2: Derivation of eigenpairs via a boundary value problem

The presentation will be a little cleaner if we remove the diagonal from A. We write $A = -2kI + kB$. For example when $n = 4$:

$$B = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad \text{so} \quad A = \begin{bmatrix} -2k & k & 0 & 0 \\ k & -2k & k & 0 \\ 0 & k & -2k & k \\ 0 & 0 & k & -2k \end{bmatrix} = -2k \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} + k \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

If $\mathbf{v}$ is an eigenvector of B with eienvalue λ, then the eigenequation $B\mathbf{v} = \lambda\mathbf{v}$ implies
$$A\mathbf{v} = (-2kI + kB)\mathbf{v} = (-2k + k\lambda)\mathbf{v}.$$

That is, $\mathbf{v}$ is an eigenvector of A with eigenvalue $-2k + k\lambda$.

With this in mind we set about deriving the eigenvalues and eigenvectors of B. Let $\mathbf{v}$ be an eigenvector of B. Write: $\mathbf{v} = \begin{bmatrix} \mathbf{v}[1] \\ \mathbf{v}[2] \\ \vdots \\ \mathbf{v}[n] \end{bmatrix}$.

The eigenequation $B\mathbf{v} = \lambda\mathbf{v}$ can be written out as

$$\begin{aligned} \mathbf{v}[2] &= \lambda\mathbf{v}[1] \\ \mathbf{v}[1] + \mathbf{v}[3] &= \lambda\mathbf{v}[2] \\ \mathbf{v}[2] + \mathbf{v}[4] &= \lambda\mathbf{v}[3] \\ &\dots \\ \mathbf{v}[n-2] + \mathbf{v}[n] &= \lambda\mathbf{v}[n-1] \\ \mathbf{v}[n-1] &= \lambda\mathbf{v}[n] \end{aligned}$$

Except for the first and last equations, all these equations look the same. We can make all the equations look the same by introducing $\mathbf{v}[0]$ and $\mathbf{v}[n+1]$:

$$\begin{aligned} \mathbf{v}[0] + \mathbf{v}[2] &= \lambda\mathbf{v}[1] \\ \mathbf{v}[1] + \mathbf{v}[3] &= \lambda\mathbf{v}[2] \\ \mathbf{v}[2] + \mathbf{v}[4] &= \lambda\mathbf{v}[3] \\ &\dots \\ \mathbf{v}[n-2] + \mathbf{v}[n] &= \lambda\mathbf{v}[n-1] \\ \mathbf{v}[n-1] + \mathbf{v}[n+1] &= \lambda\mathbf{v}[n] \end{aligned}$$

To make sure this doesn't change anything, we must require that

$$\mathbf{v}[0] = 0 \quad \text{and} \quad \mathbf{v}[n+1] = 0. \tag{BC}$$

The equations above have the form

$$\mathbf{v}[j-1] + \mathbf{v}[j+1] = \lambda\mathbf{v}[j] \quad \text{for} \quad j = 1, 2, \dots n \tag{5}$$

We rewrite them as

$$\mathbf{v}[j-1] - \lambda\mathbf{v}[j] + \mathbf{v}[j+1] = 0 \quad \text{for} \quad j = 1, 2, \dots n \tag{6}$$

This is called a difference equation for the $\mathbf{v}$.

The conditions (BC) are called boundary conditions. The name boundary conditions indicates that they are on the *boundary* or ends of the vector. Physically, $\mathbf{v}[0]$ and $\mathbf{v}[n+1]$ correspond to the pieces in ice baths at the end of the rod in positions x_0 and x_{n+1} respectively.

To summarize: we've recast the eigenequation as a difference equation with boundary conditions.

4.2.1 Solving the difference equation

Our first goal will be to solve the difference equation in Equation 6 without considering the boundary conditions. For this, we use our usual method of optimism. In the case of difference equations, we guess solutions of the form $\mathbf{v}[j] = a^j$, where a is a constant. Substituting this into Equation 6, we get

$$a^{j-1} - \lambda a^j + a^{j+1} = 0.$$

Factoring out a^{j-1}, we get the characteristic equation

$$1 - \lambda a + a^2 = 0.$$

The quadratic formula now yields $a = \dfrac{\lambda \pm \sqrt{\lambda^2 - 4}}{2}$ By reversing the order under the square root, we can write this in the form

$$a = \frac{\lambda}{2} \pm i\,\frac{\sqrt{4-\lambda^2}}{2}.$$

Now comes a clever trick: we notice that $\left(\dfrac{\lambda}{2}\right)^2 + \left(\dfrac{\sqrt{4-\lambda^2}}{2}\right)^2 = 1$. So, for $\lambda \le 2$, we can choose θ so that

$$\frac{\lambda}{2} = \cos(\theta),\ \frac{\sqrt{4-\lambda^2}}{2} = \sin(\theta),\ \text{and } a = \cos(\theta) \pm i\sin(\theta) = e^{\pm i\theta}. \tag{7}$$

Thus, we have found the following two modal solutions to the difference equation 6:

$$\mathbf{v}_1[j] = \left(e^{i\theta}\right)^j = e^{ij\theta}, \qquad \mathbf{v}_2[j] = \left(e^{-i\theta}\right)^j = e^{-ij\theta}.$$

The general solution to the difference equation is a superposition of the two modal solutions

$$\mathbf{v}[j] = c_1\mathbf{v}_1[j] + c_2\mathbf{v}_2[j] = c_1e^{ij\theta} + c_2e^{-ij\theta} \quad \text{for} \quad j = ... - 2, -1, 0, 1, 2, ...$$

(We won't go into it, but, since the characteristic equation is second-order, the space of solutions to the difference equation is two dimensional.)

4.2.2 Satisfying the boundary conditions

Notice that we solved the difference equation 6 for every value of $\lambda \le 2$. (It will turn out that this is good enough since we will find enough eigenvalues of this form.) Now we have to figure out which of these solutions also satisfy the boundary conditions (BC). Since such λ are the eigenvalues of B we know there are at most n of them.

Substituting the general solution of Equation 6 into the boundary conditions, we get

$$\begin{aligned} \mathbf{v}[0] &= c_1 + c_2 = 0 \\ \mathbf{v}[n+1] &= c_1e^{i(n+1)\theta} + c_2e^{-i(n+1)\theta} = 0 \end{aligned}$$

Solving we get

$$c_1 = -c_2 \quad \text{and} \quad e^{i(n+1)\theta} - e^{-i(n+1)\theta} = 0$$

The difference of exponentials $e^{i(n+1)\theta} - e^{-i(n+1)\theta} = 2i\sin((n+1)\theta)$. This is 0 exactly when $(n+1)\theta = m\pi$ for some integer m.

We want n distinct eigenvalues. From Equation 7 we get eigenvalues

$$\lambda_m = 2\cos(\theta_m),\ \text{ with }\ \theta_m = \frac{m\pi}{n+1}, \quad \text{for} \quad m = 1, 2, \ldots, n.$$

Converting from eigenvalues of B to eigenvalues of A, we see that the n eigenvalues of A are

$$-2k + k\lambda_m = -2k + 2k\cos(\theta_m) \quad \text{for} \quad m = 1, 2, \ldots, n.$$

Using the relation $c_1 = -c_2$ found above, the corresponding eigenvectors are

$$c_1 \left(\begin{bmatrix} e^{i\theta_m} \\ e^{i2\theta_m} \\ \vdots \\ e^{in\theta_m} \end{bmatrix} - \begin{bmatrix} e^{-i\theta_m} \\ e^{-i2\theta_m} \\ \vdots \\ e^{-in\theta_m} \end{bmatrix} \right) = c_1 \begin{bmatrix} e^{i\theta_m} - e^{-i\theta_m} \\ e^{i2\theta_m} - e^{-i2\theta_m} \\ \vdots \\ e^{in\theta_m} - e^{-in\theta_m} \end{bmatrix} = 2ic_1 \begin{bmatrix} \sin(\theta_m) \\ \sin(2\theta_m) \\ \vdots \\ \sin(n\theta_m) \end{bmatrix}$$

Removing the factor of $2ic_1$, these are exactly the eigenvectors claimed in the theorem.

We have found all the eigenpairs needed to give the general solution to the discrete heat equation $\mathbf{u}' = A\mathbf{u}$. We record it here:

$$\mathbf{u}(t) \;=\; c_1 e^{\lambda_1 t}\mathbf{v_1} + \ldots + c_n e^{\lambda_n t}\mathbf{v_n},$$

where $\theta_m = \dfrac{m\pi}{n+1}$, $\lambda_m = -2 + 2\cos(\theta_m)$, $\mathbf{v_m} = \begin{bmatrix} \sin(\theta_m) \\ \sin(2\theta_m) \\ \vdots \\ \sin(n\theta_m) \end{bmatrix}$.

5 Letting n go to infinity

The discrete model says that a given section of the heated rod has a uniform temperature. This is clearly flawed. We can make it more accurate by dividing the rod into more and more pieces. In the limit, the pieces become infinitesimal and the model becomes exact. (Well, exact assuming the linear assumptions in Newton's law of cooling are true.)

Our goal in this section is to show that, as n goes to infinity,

1. modal solutions of the discrete heat equation with boundary conditions go to modal solutions of the continuous heat equation with boundary conditions.

2. the discrete heat equation with discrete boundary conditions goes to the continuous heat equation with continuous boundary conditions.

While we proceed, you should remember that the entries in the vector $\mathbf{u}(t)$ represent the temperature at discrete postions along the rod. In the limit, the vector will become the heat function $u(x,t)$, giving the temperature at every point along the rod.

5.1 The rate constant k

Physically, it makes more sense to talk about the movement of heat content between the sections than than the movement of temperature. Since heat content is the integral of temperature we were able to write out equations in terms of temperature. But this makes the rate constant k dependent on the dimensions of the sections as well as the physical properties of the material in the rod.

We know that as Δx decreases, there is less distance for the heat to move so k should increase. Empirically, it turns out that

$$k = \frac{k_0}{(\Delta x)^2}, \tag{8}$$

where k_0 is a physical constant associated to the material but not the dimensions of the sections. (See the appendix for a derivation of Equation 8 from Fourier's law of heat conduction.)

5.2 The limit of discrete modal solutions

The goal of this section is to show that, in the limit as n goes to infinity, the modal solutions to the Equation 4 go to modal solutions of the continuous heat equation.

The computations to do this limiting procedure are a little involved, but they follow the standard methods from calculus. We have

$$\begin{aligned}
L &= \text{ length of rod} \\
\Delta x &= \frac{L}{n+1} = \text{ width of the segments} \\
x_j &= j\Delta x = \frac{jL}{n+1} = \text{ center of the } j\text{th segment} \\
\theta_m &= \frac{m\pi}{n+1} \\
\sin(j\theta_m) &= \sin\left(j \cdot \frac{m\pi}{n+1}\right) = \sin\left(\frac{m\pi}{L} \cdot x_j\right)
\end{aligned}$$

As n increases, the points $x_j = j\Delta x$ *fill in* the rod. So the vector

$$\mathbf{v_m} = \begin{bmatrix} \sin(\theta_m) \\ \sin(2\theta_m) \\ \vdots \\ \sin(n\theta_m) \end{bmatrix} = \begin{bmatrix} \sin(m\pi x_1/L) \\ \sin(m\pi x_2/L) \\ \vdots \\ \sin(m\pi x_n/L) \end{bmatrix}$$

can be replaced by the function $\sin(m\pi x/L)$.

Likewise, for the eigenvalue λ_m, we have

$$\begin{aligned}
\lambda_m &= \left(-2 + 2\cos\left(\frac{m\pi}{n+1}\right)\right) k \\
&= \left(-2 + 2\cos\left(\frac{m\pi}{n+1}\right)\right) \frac{k_0}{(\Delta x)^2} \\
&= \left(-2 + 2\cos\left(\frac{m\pi}{n+1}\right)\right) \frac{k_0(n+1)^2}{L^2}
\end{aligned}$$

Using the power series for $\cos\left(\frac{m\pi}{n+1}\right)$, this expression can be written as

$$\begin{aligned}
&= \left(-2 + 2 - \frac{2\left(\frac{m\pi}{n+1}\right)^2}{2} + \frac{2\left(\frac{m\pi}{n+1}\right)^4}{4!} - \ldots\right) \frac{k_0(n+1)^2}{L^2} \\
&= -\left(\frac{m\pi}{L}\right)^2 k_0 + \text{ terms with powers of } \frac{1}{(n+1)^2}
\end{aligned}$$

The last equality shows that, in the limit as n goes to infinity, $\lambda_m \to -\left(\frac{m\pi}{L}\right)^2 k_0$.

Putting together the limits of $\mathbf{v_m}$ and λ_m, we see that, as n goes to infinity, the modal solution to the discrete heat equation, $\mathbf{u}(t) = e^{-\lambda_m t}\mathbf{v_m}$, goes to a modal solution to the continuous heat equation

$$u(x,t) = e^{-(m\pi/L)^2 k_0 t} \sin\left(\frac{m\pi}{L}\,x\right). \tag{9}$$

5.3 The limit of the discrete heat equation

We just saw that, in the limit, solutions to the discrete heat equation go to the solutions of the continuous heat equation. We will now show that the discrete heat equation (Equation 4) limits to the continuous heat equation (Equation 1).

In the discrete heat equation, we have

$$u_j' = k(u_{j-1} - 2u_j + u_{j+1}) \quad \text{for} \quad j = 1, 2, \dots, n$$

where, just as we did above, we define $u_0(t)$ and $u_{n+1}(t)$ to have the boundary conditions

$$u_0(t) = 0 \quad \text{and} \quad u_{n+1}(t) = 0.$$

Using Equation 8 to substitute for k, we have

$$u_j' \;=\; \frac{k_0}{(\Delta x)^2}(u_{j-1} - 2u_j + u_{j+1}) \;=\; k_0 \frac{u_{j-1} - 2u_j + u_{j+1}}{(\Delta x)^2} \tag{10}$$

Since $u_j(t)$ is the temperature of the rod at $x_j = j\Delta x$ we can write $u_j(t) = u(j\Delta x, t)$. Therefore, the expression $u_{j-1} - 2u_j + u_{j+1}$ is a second difference in the x variable. That is

$$u_{j-1} - 2u_j + u_{j+1} = u((j-1)\Delta x,\, t) - 2u(j\Delta x,\, t) + u((j+1)\Delta x,\, t) \approx \frac{\partial^2 u}{\partial x^2}(j\Delta x,\, t)\cdot \Delta x^2 \tag{11}$$

Likewise

$$u_j'(t) = \frac{\partial u}{\partial t}(j\Delta x,\, t). \tag{12}$$

Using Equations 12 and 11, Equation 10 becomes

$$\frac{\partial u}{\partial t}(j\Delta x,\, t) \approx k_0 \frac{\partial^2 u}{\partial x^2}(j\Delta x,\, t)$$

Now, in the limit as n goes to infinity this equation becomes exact

$$\frac{\partial u}{\partial t}(x,t) = k_0 \frac{\partial^2 u}{\partial x^2}(x,t).$$

We have just shown that, in the limit, the discrete heat equation becomes the continuous heat equation.

Finally, in the limit, the boundary conditions become

$$u(0,\, t) = 0 \quad \text{and} \quad u(L,t) = 0.$$

6 Appendix

6.1 The empirical principle: Fourier's law of heat conduction

In Section 8.5 of their text, Edwards and Penney (*Elementary Differential Equations with Boundary Value Problems*, fifth edition) give a nice derivation of the continuous heat equation based on an empirical principle called Fourier's law of heat conduction. This law says

$$\phi(x,t) = -K\frac{\partial u}{\partial x}(x,t),$$

where ϕ is the heat flux (heat per area per time) through the cross-section at position x and time t and K is the thermal conductivity of the material. (Flux is positive from right to left.)

In our derivation of the continuous heat equation, we made use of the empirical principle $k = \frac{k_0}{(\Delta x)^2}$, where k is the rate constant in the discrete heat equation and k_0 is a physical constant associated with the material of the rod but not its dimensions.Here we will show this is equivalent Fourier's law.

To connect Fourier's law and our empirical principle, we need to know that the heat content in a section of rod from a to b is

$$Q = \int_a^b c\delta A u(x,t)\,dx$$

where c is the specific heat of the material, δ the density of the rod and A the cross-sectional area. If $\Delta x = b - a$ is small then

$$Q \approx c\delta A u(a,t)\Delta x.$$

The net heat flux into the section of rod is therefore

$$\frac{1}{A}\frac{\partial Q}{\partial t} \approx c\delta\frac{\partial u}{\partial t}(a,t)\Delta x$$

The net heat flux into the section is the difference between the fluxes at either end. So, using Fourier's law, (we have to be careful with signs):

$$\text{net flux in } = \phi(a,t) - \phi(b,t) = K\left(\frac{\partial u}{\partial x}(b,t) - \frac{\partial u}{\partial x}(a,t)\right) \approx K\frac{\partial^2 u}{\partial x^2}(a,t)\,\Delta x.$$

Equating these two formulas for net flux we get

$$c\delta\frac{\partial u}{\partial t}(a,t)\Delta x \approx K\frac{\partial^2 u}{\partial x^2}(a,t)\,\Delta x. \tag{13}$$

Now we approximate the second partial derivative by a second difference

$$\frac{\partial^2 u}{\partial x^2}(a,t) \approx \frac{u(a-\Delta x,\,t) - 2u(a,t) + u(a+\Delta x,\,t)}{\Delta x^2}$$

Equation 13 becomes

$$\begin{aligned}\frac{\partial u}{\partial t}(a,t) &\approx \frac{K}{c\delta}\frac{\partial^2 u}{\partial x^2}(a,t)\\ &\approx \frac{K}{c\delta}\frac{u(a-\Delta x,\,t)-2u(a,t)+u(a+\Delta x,\,t)}{\Delta x^2}\\ &= \frac{K}{c\delta(\Delta x)^2}(u(a-\Delta x,\,t)-2u(a,t)+u(a+\Delta x,\,t))\end{aligned}$$

Now if $a = x_j$, $a - \Delta x = x_{j-1}$ and $a + \Delta x = x_{j+1}$ then this becomes our discrete heat equation

$$\frac{\partial u}{\partial t}(x_j,t) \approx \frac{K}{c\delta(\Delta x)^2}(u(x_{j-1},\,t)-2u(x_j,\,t)+u(x_{j+1},\,t))$$

Comparing constants, we see that $k = \frac{K}{c\delta(\Delta x)^2}$, so letting $k_0 = \frac{K}{c\delta}$ we get

$$k = \frac{k_0}{\Delta x^2}$$

which is exactly the principle we asserted.