An Introduction to Partial Differential Equations

Andrew J. Bernoff

LECTURE 2
Cooling of a Hot Bar: The Diffusion Equation

2.1. Outline of Lecture

- An Introduction to Heat Flow
- Derivation of the Diffusion Equation
- Examples of Solution to the Diffusion Equation
- The Maximum Principle
- Energy Dissipation and Uniqueness

2.2. An Introduction to Heat Flow

A classical example of the application of ordinary differential equations is Newton's Law of Cooling which, basically, answers the question *"How does a cup of coffee cool?"* Newton hypothesized that the rate at which the temperature, $U(t)$, changes is proportional to the difference with the ambient temperature, which we call $\bar{U}$,

$$\frac{dU}{dt} = -\kappa(U - \bar{U}). \tag{2.1}$$

Here κ is a positive rate constant (with units of inverse time) that measures how fast heat is lost from the coffee cup to the ambient environment. If we specify the initial temperature,

$$U(0) = U_0, \tag{2.2}$$

we can solve for the evolution of the temperature,

$$U(t) = \bar{U} + (U_0 - \bar{U})e^{-\kappa t}. \tag{2.3}$$

Figure 2.1: (a) A coffee cup (b) Its temperature as a function of time. (draw your own figure).

If we graph the temperature as a function of time, we see that it decays exponentially to the ambient temperature, $\bar{U}$, at a rate governed by κ.

When we derived Newton's Law of cooling we made several assumptions – most importantly that the temperature in the coffee cup did not vary with location. If we account for the variation of temperature with location, we can derive a PDE called the **heat equation** or, more generally, the **diffusion equation**. If the temperature, $U(x,t)$ is a function of a single spatial variable, x, we will show that it satisfies the diffusion equation,

$$U_t = DU_{xx},$$

where D is a constant known as the thermal diffusivity. In higher dimensions, the equation can be written

$$U_t = D\nabla^2 U,$$

where ∇^2 is the **Laplacian**.

2.3. Derivation of the Diffusion Equation

The diffusion equation will be our second example of a conservation law; we can derive the equation by accounting for the flow of thermal energy. Suppose we consider a metal bar, with a uniform cross-sectional area, A, whose temperature, $U(x,t)$, is a function of time, t, and the position, x, along the bar (that is we assume the temperature is uniform in every cross-section).

Figure 2.2: Conservation of heat in a metal bar
of cross-sectional area A.
(draw your own figure).

Let the thermal energy in the region $a < x < b$ is given by

$$\mathcal{E} = \rho_0 c_v A \int_a^b U(x,t)\, dx \tag{2.4}$$

The important term in the integral is the temperature, $U(x,t)$, measured in degrees. The remaining constants, A, the cross-sectional area (with units of [(length)^2]), ρ_0, the density [mass/(length)^3] and c_v, the heat capacity [energy/(degree $\cdot$ mass)] are physical properties of the material – think of them as being obligatory for making the units work out.

We wish to equate the change in thermal energy to the heat flux out of the bar through the planes at $x = a$ and $x = b$. To do this we use **Fourier's heat law** which states that the flux density of thermal energy, $q(x,t)$ is proportional to the temperature gradient,

$$q(x,t) = -kU_x, \tag{2.5}$$

where the negative sign reflects the fact that heat flows from hot to cold, just as in Newton's law of cooling, with a constant of proportionality, k, called the thermal conductivity [(energy$\cdot$length)/(degrees$\cdot$time)].

Figure 2.3: Heat flux is from hot to cold!!
(draw your own figure).

Now, the total flux of thermal energy into the **into** the region $a < x < b$ is given by

$$Q = A[q(a,t) - q(b,t)], \tag{2.6}$$

where we multiply by the area A to get the total flux through the cross-section.

By **conservation of energy**, the rate of change of the energy between a and b is given by the flux into the region,

$$\frac{d\mathcal{E}}{dt} = Q. \tag{2.7}$$

Once again we can rewrite the flux by a clever application of the fundamental theorem of calculus,

$$Q = A[q(a,t) - q(b,t)] = -\, Aq(x,t)|_{x=a}^{x=b} \tag{2.8}$$

$$= -A\int_a^b q_x \; dx. \tag{2.9}$$

We now rewrite the conservation of energy equation as

$$\frac{d\mathcal{E}}{dt} = \frac{d}{dt}\left[\rho c_v A \int_a^b U \; dx\right] = \int_a^b \rho c_v A U_t \; dx = Q = -A\int_a^b \; q_x dx, \tag{2.10}$$

or, rearranging

$$\int_a^b \rho c_v A\, U_t + A q_x \, dx = 0. \tag{2.11}$$

Since this is true for **every** interval $a < x < b$, the integrand must vanish identically. So

$$\rho c_v A U_t + A q_x = 0. \tag{2.12}$$

Substituting for the flux function $q(x,t) = -kU_x$ yields

$$\rho c_v A U_t - kA(U_x)_x = 0. \tag{2.13}$$

Rearranging the equation yields the diffusion equation,

$$\boxed{U_t = D U_{xx},} \tag{2.14}$$

where the **diffusivity**, $D = k/(\rho c_v)$, is a constant which is determined by the geometry and physical properties of the metal bar.

To complete the description of the problem, we need to supplement the diffusion equation with boundary conditions and initial conditions. Suppose we consider a bar of finite length L, occupying the region $0 < x < L$. At the boundaries of the metal bar we can specify a fixed temperature,

$$U(0,t) = U_0 \qquad U(L,t) = U_1, \tag{2.15}$$

which are usually referred to as **Dirichlet** boundary conditions. Alternatively, we could specify a heat flux,

$$q_0 = q(0,t) = -kU_x(0,t) \qquad q_1 = q(L,t) = -kU_x(L,t). \tag{2.16}$$

Specifying the gradient across the boundary is referred to as **Neumann** boundary conditions.

Finally, we also need to specify the initial temperature distribution,

$$U(x,0) = f(x) \qquad 0 < x < L. \tag{2.17}$$

We will demonstrate below that the solution to this problem (if it exists) is unique; later in this course we will solve this problem using the method of separation variables.

For completeness, we also comment here that the problem can be posed on the infinite line, $-\infty < x < \infty$ sometime called the **Cauchy** problem – in this case one usually replaces the boundary condition with the specification that the temperature remains bounded as we approach infinity,

$$\lim_{x \to \pm\infty} |U(x,t)| < C, \tag{2.18}$$

for some constant C. This condition may seem superfluous at first glance, but actually is necessary to stop heat from leaking in from infinity (speaking very, very informally an infinite source of heat infinitely far away can have a finite effect in a short amount of time). If you are interested in details, look for the examples of Tychonov in a PDE's text[1].

2.4. Examples of Solution to the Diffusion Equation

We can summarize the last section by restating a well-posed problem for the diffusion equation on the interval $0 < x < L$ with Dirichlet boundary conditions,

The Dirichlet Problem for the Diffusion Equation
(Non-homogeneous Boundary Conditions)

$$\begin{array}{rlcl} & U_t = DU_{xx} & 0 < x < L, t > 0 & \text{DE} \\ U(0,t) = U_0 & U(L,t) = U_1 & t > 0 & \text{BC} \\ & U(x,0) = f(x) & 0 < x < L. & \text{IC} \end{array}$$

Solving the general problem will have to wait, but we can find some specific solutions to the problem using the ideas of **Separation of Variables**. For the moment, we will restrict ourselves to homogeneous boundary conditions,

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

$$\begin{array}{rlcl} & U_t = DU_{xx} & 0 < x < L, t > 0 & \text{DE} \\ U(0,t) = 0 & U(L,t) = 0 & t > 0 & \text{BC} \\ & U(x,0) = f(x) & 0 < x < L, & \text{IC} \end{array}$$

If you want, you can skip the derivation for the moment and jump ahead to Exercise 1, if you don't mind the solution appearing *deus ex machina* (a fancy term for "out of thin air").

[1]See, for example, T. W. Körner, "Fourier Analysis," Cambridge University Press, p. 338.

2.4.1. A Solution to the Homogeneous Dirichlet Problem

Let us look for solutions to the homogeneous Dirichlet problem of the form

$$U(x,t) = X(x)T(t) \tag{2.19}$$

we find from the differential equation (DE) that

$$XT_t = DX_{xx}T \tag{2.20}$$

and dividing by XT we find

$$\frac{T_t}{DT} = \frac{X_{xx}}{X} = -\lambda. \tag{2.21}$$

where λ is to be determined. Now because T_t/DT is **only** a function of t and X_{xx}/X is **only** a function of x we know that λ must be independent of x and t respectively, and therefore must be a constant – consequently it is known as the **separation constant**. We can now solve the resulting ODE for $T(t)$

$$T_t = -\lambda DT \quad \Rightarrow \quad T(t) = e^{-\lambda t}, \tag{2.22}$$

or some constant multiple of it.

We now look for a solution for the $X(x)$ equation that also satisfies the homogeneous boundary conditions. From the boundary conditions (BC), we know that

$$U(0,t) = X(0)T(t) = 0 \quad \Rightarrow \quad X(0) = 0 \tag{2.23}$$

$$U(0,t) = X(L)T(t) = 0 \quad \Rightarrow \quad X(L) = 0 \tag{2.24}$$

So finally we conclude that we are looking for solutions to the **Boundary Value Problem** for $X(x)$,

$$\boxed{X_{xx} + \lambda X = 0, \qquad X(0) = 0 \quad X(L) = 0.} \tag{2.25}$$

Solving the DE, we find that

$$X(x) = B\cos(\sqrt{\lambda}x) + C\sin(\sqrt{\lambda}x) \tag{2.26}$$

and applying the boundary conditions we see that $X(0) = 0$ implies that $B = 0$, and that

$$C\sin(\sqrt{\lambda}L) = 0. \tag{2.27}$$

Consequently, a non-trivial solution (that is a solution for which $X(x) \neq 0$) for $X(x)$ can be found if and only if

$$\boxed{\lambda = \lambda_n \equiv \left(\frac{n\pi}{L}\right)^2 \quad \text{for} \quad n = 1, 2, 3\ldots} \tag{2.28}$$

for which we find

$$X(x) = X_n(x) \equiv \sin\left(\frac{n\pi x}{L}\right) \quad \text{for} \quad n = 1, 2, 3 \ldots, \tag{2.29}$$

or some constant multiple of it. These special values of λ are called **eigenvalues** and the associated functions, $X_n(x)$, are known as **eigenfunctions**.

Multiplying the solution for $X_n(x)$ and $T(t)$ together finally yields a solution for $U_n(x, t)$,

$$U(x, t) = U_n(x, t) \equiv \sin\left(\frac{n\pi x}{L}\right) e^{-\left(\frac{n\pi}{L}\right)^2 Dt} \text{ for } n = 1, 2, 3 \ldots. \tag{2.30}$$

The method of separation of variables is very powerful – it will be one of our primary tools for finding solutions to PDE's in the coming lectures.

Exercise 1. Verify that

$$U_n(x, t) \equiv \sin\left(\frac{n\pi x}{L}\right) e^{-\left(\frac{n\pi}{L}\right)^2 t} \quad \text{for} \quad n = 1, 2, 3 \ldots,$$

satisfies the diffusion equation $U_t = DU_{xx}$ and the homogeneous boundary conditions $U(0, t) = U(L, t) = 0$. Explain why any linear combination of U_n,

$$U(x, t) = \sum_{n=1}^{\infty} a_n U_n(x, t) = \sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi x}{L}\right) e^{-\left(\frac{n\pi}{L}\right)^2 Dt}$$

also satisfies the diffusion equation and the homogeneous boundary condition. Does it worry you that this is an infinite sum? What initial condition, $U(x, 0)$, does this correspond to?

2.4.2. A Solution to the Cauchy Problem

We can also consider a solution to the Cauchy problem for the diffusion equation, which you hopefully remember is the problem posed on the entire real line,

THE CAUCHY PROBLEM FOR THE DIFFUSION EQUATION

$$\begin{array}{rcl} U_t = DU_{xx} & -\infty < x < \infty, t > 0 & \text{DE} \\ \lim\limits_{x\to\pm\infty} |U(x,t)| < C & t > 0, & \text{BC} \\ U(x,0) = f(x) & -\infty < x < \infty. & \text{IC} \end{array}$$

While there are many clever derivation for the solution to this problem, for the moment I will simply give you the most important solution, usually called the **fundamental solution** or the **diffusion kernel**,

$$U(x,t) = G(x,t+\tau) \equiv \frac{1}{\sqrt{4\pi D(t+\tau)}} e^{-\frac{x^2}{4D(t+\tau)}}. \tag{2.31}$$

where τ is a constant (which we will assume is positive). This solution can be used to construct a general solution of the diffusion equation for an arbitrary initial condition, $f(x)$.

Exercise 2. Verify that

$$G(x,t+\tau) \equiv \frac{1}{\sqrt{4\pi D(t+\tau)}} e^{-\frac{x^2}{4D(t+\tau)}}.$$

satisfies the diffusion equation and the boundary conditions for the Cauchy problem when $\tau > 0$. Show that this solution corresponds to a Gaussian with time varying width and height. How does the Gaussian's width, height and area vary in time?

2.5. The Maximum Principle

Looking at solutions to the heat equation, we note that they tend to average out maximums and minimums. We can develop some intuition for this by considering what the equation says. Basically, $U_t = DU_{xx}$ means: *The temperature is decreasing when the profile is convex down and the temperature is increasing when the profile is convex up.*

Figure 2.4: The heat equation interperted graphically
(draw your own figure).

From which we conclude that interior maximums in temperature are decreasing and interior minimums of temperature are increasing. This reasoning is not quite airtight (how to make it tighter is a good question to ponder). We can give a rigorous statement (without proof) of the maximum principle:

Theorem 2.32 (Maximum Principle for the Diffusion Equation)**.** *If $u(x,t)$ satisfies the Dirichlet problem for the diffusion equation in the semi-infinite strip $0 < x < L$, $0 < t$, then it assumes its maximum value (as a function of x and t) either initially (when $t = 0$) or on the lateral boundaries (where $x = 0$ or $x = l$).*

The same is also true of the minimum of $u(x,t)$. A proof can be found in most advanced PDE texts.

Exercise 3. Interpret the solutions we have found for the diffusion equation in terms of the maximum principle. Show examples where the maximum value of $u(x,t)$ occur in the initial condition and on the lateral boundaries.

2.6. Energy Dissipation and Uniqueness

By looking at what is normally known as energy for the diffusion equation, we can show that the solution for the Dirichlet problem is unique. Note this energy is a mathematical construct, not to be confused with the thermal energy discussed in the derivation of the diffusion equation.

First, suppose that $U(x,t)$ is a solution to the homogeneous Dirichlet problem,

$$\begin{array}{rlll} & U_t = DU_{xx} & 0 < x < L, t > 0 & \text{DE} \\ U(0,t) = 0 & U(L,t) = 0 & t > 0 & \text{BC} \\ & U(x,0) = f(x) & 0 < x < L, & \text{IC} \end{array}$$

Let's define, the energy,

$$W = \frac{1}{2}\int_0^L U^2 \, dx, \tag{2.33}$$

which is a function of t dependent on the particular solution $U(x,t)$ (technically it is a function of t and a **functional** of $U(x,t)$). Note that $W \geq 0$ with $W = 0$ only for the trivial solution $U(x,t) = 0$.

If we differentiate the energy with respect to time, we find

$$\begin{aligned} \frac{dW}{dt} &= \int_0^L UU_t \, dx, \\ &= D\int_0^L UU_{xx} \, dx, \\ &= -\int_0^L (U_x)^2 \, dx + UU_{xx} \big|_{x=0}^{x=L}, \end{aligned}$$

where we have substituted the DE and used integration by parts. Now, applying the BC's, we fine that the boundary terms from the integration by parts vanish, so,

$$\frac{dW}{dt} = -\int_0^L (U_x)^2 \, dx \leq 0$$

Now, we can conclude that W is decreasing (that is energy is dissipated!!)**unless** $U_x = 0$, that is to say that U is constant. As the only constant solution satisfying the boundary conditions is $U = 0$, we might be tempted to conclude that the solution always decays to this trivial state. This turns out to be true, although one must invest some analysis to show it rigorously.

Figure 2.4: (a) A solution to the homogeneous Dirichlet problem for the heat equation. (b) The corresponding energy, W, which is decreasing to zero.
(draw your own figure).

A second conclusion one can reach is that if $f(x) = 0$, that $U(x,t) = 0$ for all $t > 0$. This follows quickly because $W = 0$ at $t = 0$, it is non-increasing and non-negative. While this seems like a trivial result, it has a very powerful consequence. Suppose we had two solutions to the non-homogeneous Dirichlet problem, call them V_1 and V_2. You should be able to convince yourself that there difference $U = V_1 - V_2$ satisfies the homogeneous Dirichlet problem with $f(x) = 0$. Consequently, we know that $U(x,t) = 0$ for all $t > 0$, which implies $V_1 = V_2$. From this we conclude that *The solution to the non-homogeneous Dirichlet problem is unique*, a powerful result indeed.

Exercise 4. Convince yourself the energy argument for uniqueness of solutions in the previous paragraph is correct. Show that a similar argument can be made for the Neumann problem.

2.7. Challenge Problems for Lecture 2

Problem 1. Consider the diffusion equation with homogeneous Neumann boundary conditions.

$$\begin{array}{llll} & U_t = DU_{xx} & 0 < x < L, t > 0, & \text{DE} \\ U_x(0,t) = 0 & U_x(L,t) = 0 & t > 0, & \text{BC} \\ & U(x,0) = f(x) & 0 < x < L. & \text{IC} \end{array}$$

(a) Explain physically why this corresponds to the diffusion of heat in a metal bar with insulated ends. Make sure you understand what each of the equations corresponds to.

(b) Show that

(i) $U_0(x,t) = 1$

(ii) $U_n(x,t) = \cos\left(\frac{n\pi x}{L}\right) e^{-\left(\frac{n\pi}{L}\right)^2 Dt} \qquad n = 1, 2, 3, \ldots$

satisfy both the diffusion equation (DE) and the homogeneous Neumann boundary conditions (BC).

(c) Write down a general solution as a linear combination of the solutions you found in part (b). What does this say about $f(x)$ if we assume that this solution also satisfies the initial condition (IC)?

Problem 2. In this problem, we will argue that for the homogeneous Neumann problem discussed in Problem 1, that the solution approaches a constant temperature, given by the average of the initial temperature.

(a) Suppose we define the total heat energy in the bar as

$$Q(t) = \int_0^L U(x,t)\, dx.$$

Show that Q is **conserved**, that is that it is independent of time (Hint: compute $\frac{dQ}{dt}$).

(b) Use the initial condition to compute Q in terms of $f(x)$.

(c) Modify the energy argument in the previous section show that the energy is decreasing unless $U(x,t)$ is constant. Use this to argue that $U(x,t)$ approaches a constant solution as $t \to \infty$.

(d) Finally, use parts (a) and (b) of the problem to show that there is only one possible constant solution for U that is consistent with the conservation of Q. Show that solution corresponds to the bar approaching the average temperature of the initial condition.

Problem 3. Previously we showed that the diffusion kernel,

$$U(x,t) = G(x,t+\tau) \equiv \frac{1}{\sqrt{4\pi D(t+\tau)}} e^{-\frac{x^2}{4D(t+\tau)}},$$

satisfies the diffusion equation with an initial condition

$$U(x,0) = G(x,\tau).$$

(a) Show that the total heat ,

$$Q(t) = \int_{-\infty}^{\infty} U(x,t)\ dx,$$

is conserved, and in fact $Q(t) = 1$, for the heat kernel.

(b) Show that as $\tau \to 0$, that $G(x,\tau) \to 0$ for $x \neq 0$ and that $G(0,\tau) \to \infty$.

(c) Explain why the solution $G(x,t)$ (i.e. with $\tau = 0$) corresponds to introducing a unit amount of heat concentrated at the origin when $t = 0$. This is called a δ-*function* initial condition.

Problem 4. A curious property of the diffusion equation is that both derivatives and integrals of solution satisfy the diffusion equation also. This can be used to generate new solutions from existing ones.

(a) Show that if $U(x,t)$ satisfies the diffusion equation then $\psi(x,t) = U_x$ satisfies the diffusion equation also (Hint: differentiate both sides of the diffusion equation with respect to x).

(b) Generate a new solution for the heat equation by differentiating the heat kernel with respect to x. Graph this solution (MAPLE may be useful here) – what does it look like?

(c) Show that if $\psi(x,t)$ satisfies the heat equation, then so does $U(x,t) = \int_{x_0}^{x} \psi(\xi,t)\ d\xi$.

(d) Show that

$$U(x,t) = \frac{1}{2} + \frac{1}{\sqrt{\pi}} \int_0^{x/\sqrt{4Dt}} e^{-z^2}\ dz$$

satisfies the heat equation, by showing its derivative is the heat kernel. Graph the solution at various times – what physical problem does this solution correspond to ?