Math 5587 – Lecture 4

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1 Fundamental solution of the heat equation

Consider the heat equation on the whole real line

$$u_t - ku_{xx} = 0 \quad \text{for} \quad -\infty < x < \infty. \tag{1}$$

We cannot so easily factor the equation as we did with the wave equation to derive d'Alembert's formula. Instead, we need to be slightly more clever. Notice that if $u(x,t)$ is any solution of the heat equation (1), then

$$v(x,t) := u(\alpha x, \alpha^2 t)$$

is also a solution for any real number α. To check this, we just compute

$$v_{xx}(x,t) = \alpha^2 u_{xx}(\alpha x, \alpha^2 t), \quad \text{and} \quad v_t(x,t) = \alpha^2 u_t(\alpha x, \alpha^2 t),$$

and use the fact that u solves the heat equation (1) to find that

$$v_t - kv_{xx} = \alpha^2 (u_t - ku_{xx}) = 0.$$

We have discovered a *scale invariance* in the heat equation. The different powers on α in the x and t coordinates reflect the fact that the equation is second order in x and first order in t.

It makes sense to look for a solution of the heat equation that is invariant under such a scaling. Thus, we might look for a solution $u(x,t)$ of the form

$$u(x,t) = g\left(\frac{x}{\sqrt{t}}\right), \tag{2}$$

for some yet to be determined function g. Then

$$u(\alpha x, \alpha^2 t) = g\left(\frac{\alpha x}{\sqrt{\alpha^2 t}}\right) = g\left(\frac{x}{\sqrt{t}}\right) = u(x,t)$$

for any positive real number α. Our "educated guess" as to the form of u in (2) is called an *ansatz*, and is a common technique for finding special solutions of PDE.

Now, the total amount of heat in the system must be conserved, so we require that

$$H(t) = \int_{-\infty}^{\infty} u(x,t)\, dx \quad \text{is constant in } t.$$

For our ansatz (2) we have

$$H(t) = \int_{-\infty}^{\infty} g\left(\frac{x}{\sqrt{t}}\right)\, dx = \sqrt{t}\int_{-\infty}^{\infty} g(y)\, dy, \tag{3}$$

where we made the change of variables $y = x/\sqrt{t}$ in the last step. Unfortunately the total heat is not constant, and actually grows with t, so our ansatz (2) cannot be a solution of the heat equation no matter what we choose for g.

All is not lost, however. The computation of the total heat in (3) suggests that we should instead consider the ansatz

$$u(x,t) = \frac{1}{\sqrt{t}} g\left(\frac{x}{\sqrt{t}}\right). \tag{4}$$

Then we have

$$H(t) = \frac{1}{\sqrt{t}}\int_{-\infty}^{\infty} g\left(\frac{x}{\sqrt{t}}\right)\, dx = \int_{-\infty}^{\infty} g(y)\, dy,$$

which is independent of t! Now that our ansatz is consistent with the physics of heat diffusion, let's plug u into the heat equation and see if we can deduce the function g. Notice we have

$$u_{xx}(x,t) = t^{-\frac{3}{2}} g''\left(\frac{x}{\sqrt{t}}\right),$$

and

$$u_t(x,t) = -\frac{1}{2} t^{-\frac{3}{2}}\left[g\left(\frac{x}{\sqrt{t}}\right) + g'\left(\frac{x}{\sqrt{t}}\right)\frac{x}{\sqrt{t}}\right].$$

Substituting these expressions into the heat equation $u_t - ku_{xx} = 0$ we find that

$$kg''(y) + \frac{1}{2}g(y) + \frac{1}{2}yg'(y) = 0,$$

where $y = x/\sqrt{t}$. Thus, our ansatz (4) has reduced the problem of solving a PDE to that of solving an ODE, which is generally much easier. Notice we can write this ODE as

$$g''(y) + \frac{1}{2k}(yg(y))' = 0.$$

Therefore

$$g'(y) + \frac{y}{2k}g(y) = C$$

for some constant C. Since we are only looking for one solution of the heat equation (at the moment), we can choose any value of C we like, so let's set $C = 0$. We multiply by the integrating factor $e^{y^2/4k}$ to find that

$$\frac{d}{dy}\left(e^{y^2/4k} g(y)\right) = 0.$$

and hence

$$g(y) = Ae^{-y^2/4k},$$

for any constant A. Recalling the form of the ansatz (4)

$$u(x,t) = \frac{A}{\sqrt{t}} e^{-x^2/4kt} \tag{5}$$

is a solution of the heat equation (1) for $-\infty < x < \infty$ and $t > 0$. You can (and should) check this statement by substituting $u(x,t)$ into the heat equation (1). Notice the solution is undefined when $t \leq 0$.

We usually choose $A > 0$ so that the total heat is one, i.e.,

$$\frac{A}{\sqrt{t}} \int_{-\infty}^{\infty} e^{-x^2/4kt}\, dx = \int_{-\infty}^{\infty} u(x,t)\, dx = 1.$$

Making the substitution $y = x/\sqrt{4kt}$ we require

$$A\sqrt{4k} \int_{-\infty}^{\infty} e^{-y^2}\, dy = 1.$$

We claim that

$$\int_{-\infty}^{\infty} e^{-y^2}\, dy = \sqrt{\pi}, \tag{6}$$

so that

$$A = \frac{1}{\sqrt{4\pi k}}.$$

To see why (6) holds, we square the integral and convert the problem into polar coordinates:

$$\begin{aligned}
\left(\int_{-\infty}^{\infty} e^{-y^2}\, dy\right)^2 &= \left(\int_{-\infty}^{\infty} e^{-x^2}\, dx\right)\left(\int_{-\infty}^{\infty} e^{-y^2}\, dy\right) \\
&= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-(x^2+y^2)}\, dx\, dy \\
&= \int_{0}^{2\pi}\int_{0}^{\infty} re^{-r^2}\, dr\, d\theta = -\pi e^{-r^2}\Big|_0^{\infty} = \pi.
\end{aligned}$$

Finally, our solution of the heat equation is

$$\boxed{\Phi(x,t) = \frac{1}{\sqrt{4k\pi t}} e^{-x^2/4kt}.} \tag{7}$$

This solution turns out to be very special, so we call it the *fundamental solution* of the heat equation. It is also called the *source function* or *Gaussian kernel*. The fundamental solution of the heat equation has the following important properties:

1. $\Phi_t(x,t) - k\,\Phi_{xx}(x,t) = 0$ for all x and all $t > 0$,
2. $\Phi(x,t) > 0$ for all x and all $t > 0$,
3. $\int_{-\infty}^{\infty} \Phi(x,t)\, dx = 1$ for all $t > 0$, and
4. Φ is infinitely differentiable in both x and t in its domain of definition ($t > 0$).

The fundamental solution $\Phi(x,t)$ starts off as a tall spike centered around the origin when t is small. As time increases, the height decreases and the width increases, all the while preserving the total area under the graph to be 1 (property 3 above). The height of Φ scales with $1/\sqrt{t}$ while the width scales like $\sqrt{t}$. See Figure 1 for an illustration. In probability, the function Φ is the normal or Gaussian distribution with standard deviation $\sigma = \sqrt{2kt}$.

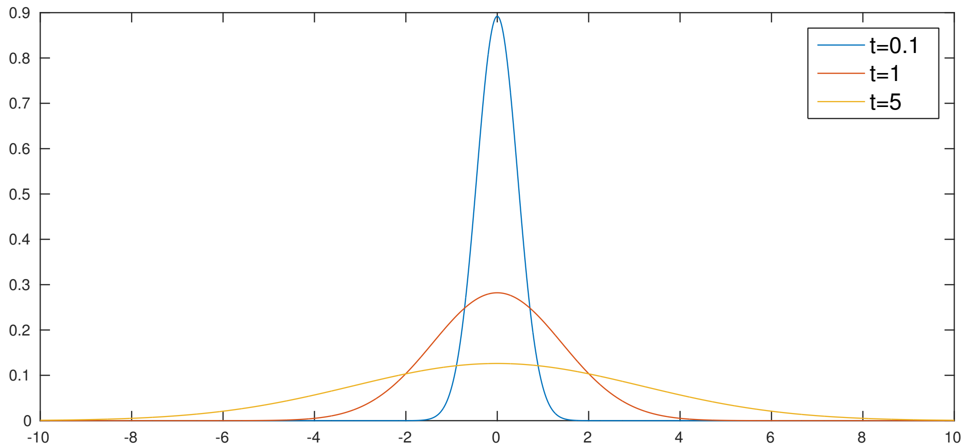


Figure 1: Plots of the fundamental solution of the heat equation with with $k = 1$ and $t = 0.1, 1, 5$.

1.1 Solving the heat equation on the whole line

Since the heat equation is translation invariant, the shifted function $\Phi(x - y, t)$ is also a solution of the heat equation for every real number y. Since the heat equation is linear, the linear combination of translated solutions

$$u(x,t) = \sum_{i=1}^{n} \Phi(x - y_i, t) f_i$$

is also a solution of the heat equation for any real numbers $y_1, \ldots, y_n$ and $f_1, \ldots, f_n$. Interpreting the sum above as a Riemann sum for an integral, it is natural to expect that

$$\boxed{u(x,t) = \int_{-\infty}^{\infty} \Phi(x - y, t) f(y)\, dy} \tag{8}$$

is a solution of the heat equation, for any reasonable function $f(y)$. Indeed, we can easily check that u solves the heat equation by differentiating under the integral to find that

$$u_t(x,t) = \int_{-\infty}^{\infty} \Phi_t(x - y, t) f(y)\, dy \quad \text{and} \quad u_{xx}(x,t) = \int_{-\infty}^{\infty} \Phi_{xx}(x - y, t) f(y)\, dy.$$

Therefore

$$u_t(x,t) - k u_{xx}(x,t) = \int_{-\infty}^{\infty} (\Phi_t(x - y, t) - k\Phi_{xx}(x - y, t)) g(y)\, dy = 0$$

since $\Phi(x - y, t)$ solves the heat equation $\Phi_t - k\Phi_{xx} = 0$.

In fact, the function u given by (8) is the solution of the heat equation

$$u_t - k u_{xx} = 0 \quad \text{for} \quad -\infty < x < \infty,$$

with initial condition $u(x,0) = f(x)$. To see why, note that Equation (8) expresses $u(x,t)$ as an average of the values of $f(y)$, weighted by the shifted fundamental solution $\Phi(x-y,t)$. As $t \to 0$, the weights become highly concentrated around $x = y$ (see Figure 1), and we recover $f(x)$ in the limit as $t \to 0^+$. More precisely we have

$$\lim_{t\to 0^+} u(x,t) = \lim_{t\to 0^+} \int_{-\infty}^{\infty} \Phi(x-y,t)f(y)\,dy = f(x)$$

whenever f is continuous at x. We will not prove this right now, but will return to this later in the course when we discuss delta functions and generalized functions[1]

The representation formula (8) justifies calling Φ the *fundamental solution* of the heat equation, since *any* solution with (reasonably) arbitrary initial condition $u(x,0) = f(x)$ can be expressed in terms of Φ.

Example 1.1. Let us find the solution $u(x,t)$ of the heat equation

$$u_t - ku_{xx} = 0 \quad \text{for } -\infty < x < \infty,$$

subject to the step function initial condition

$$f(x) = u(x,0) = \begin{cases} 1, & \text{if } x > 0 \\ 0, & \text{if } x \le 0. \end{cases}$$

The representation formula (8) yields

$$u(x,t) = \frac{1}{\sqrt{4k\pi t}} \int_0^{\infty} e^{-(x-y)^2/4kt}\,dy = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{x/\sqrt{4kt}} e^{-z^2}\,dz = \frac{1}{2} + \frac{1}{2}\mathrm{erf}\left(\frac{x}{\sqrt{4kt}}\right), \tag{9}$$

where erf is the *error function* defined by

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-z^2}\,dz.$$

There is unfortunately no closed form expression for the error function, so we are left to numerically evaluate the solution $u(x,t)$ at this point. See Figure 2 for a depiction of how the solution $u(x,t)$ evolves over time.

Example 1.2. Let us find the solution $u(x,t)$ of the heat equation

$$u_t - ku_{xx} = 0 \quad \text{for } -\infty < x < \infty,$$

subject to the initial condition $f(x) = u(x,0) = e^{-x}$. The representation formula (8) yields

$$u(x,t) = \frac{1}{\sqrt{4\pi kt}} \int_{-\infty}^{\infty} e^{-(x-y)^2/4kt} e^{-y}\,dy.$$

This is one of the fortunate few examples that can be integrated. Notice the exponent in the integrand is

$$-\frac{x^2 - 2xy + y^2 + 4kty}{4kt}.$$

[1] $\Phi(x,t)$ converges to a delta function as $t \to 0^+$, and it is common for this reason to write $\Phi(x,0) = \delta(x)$.

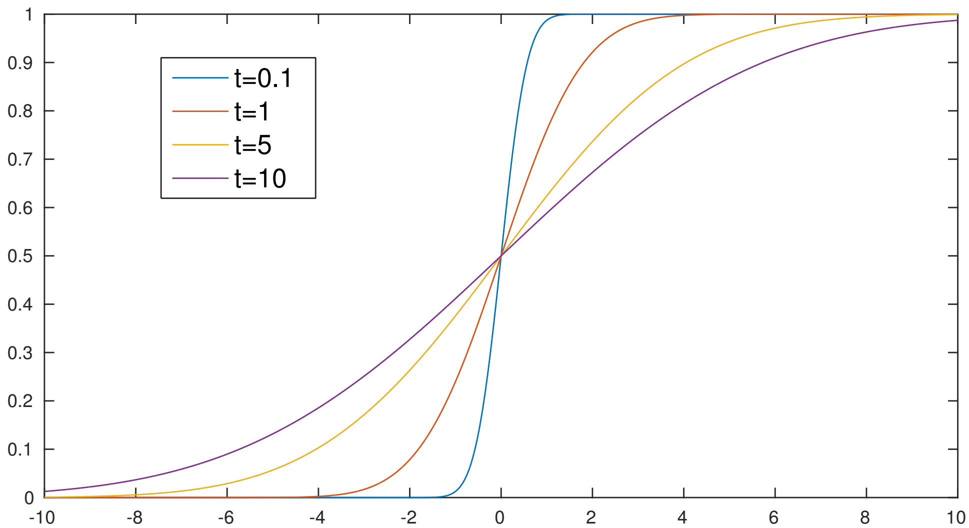


Figure 2: Plots of the solution $u(x,t) = \frac{1}{2} + \frac{1}{2}\text{erf}\left(\frac{x}{\sqrt{4t}}\right)$ at $t = 0.1, 1, 5, 10$ from Example 1.1.

We can complete the square to find that

$$-\frac{x^2 - 2xy + y^2 + 4kty}{4kt} = -\frac{(y + 2kt - x)^2}{4kt} + kt - x.$$

Make the change of variables $z = (y + 2kt - x)/\sqrt{4kt}$, so that $dy = \sqrt{4kt}dz$ and we have

$$u(x,t) = e^{kt-x}\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-z^2}\,dz = e^{kt-x}.$$

It is easy to verify that $u(x,t) = e^{kt-x}$ is indeed a solution of the heat equation.

1.2 Properties of the heat equation

We can deduce many important properties of the heat equation from the representation formula (8).

1. As we expect from physics, the total amount of heat is conserved. Indeed

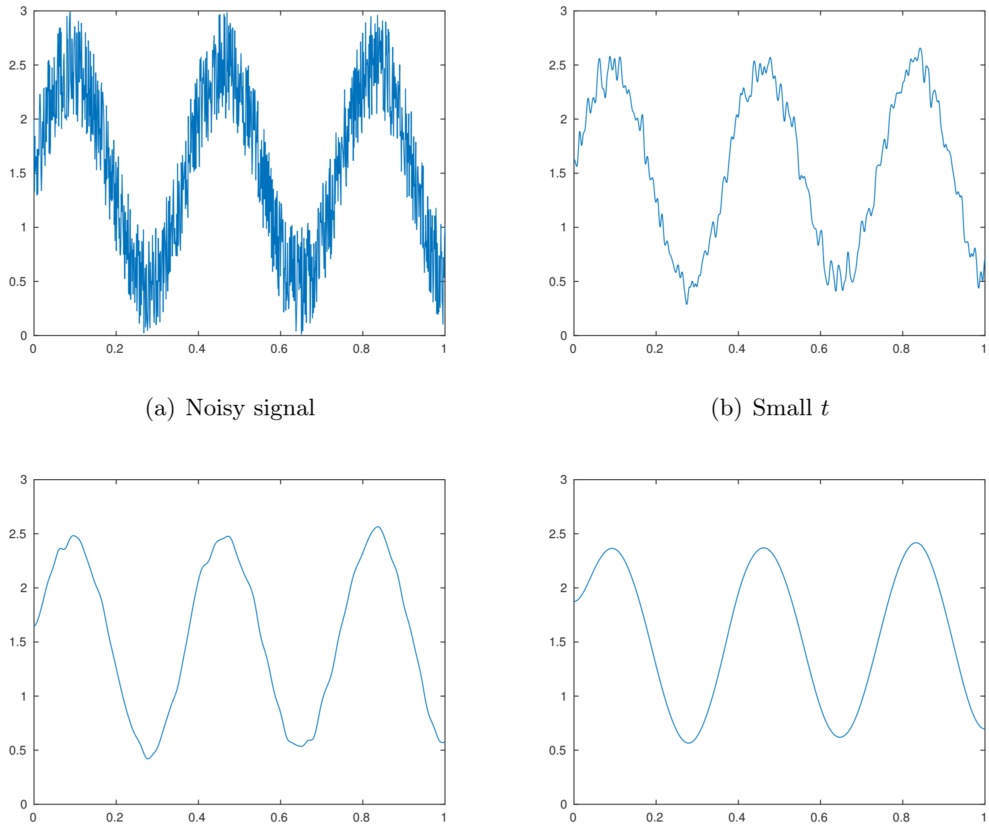
$$\text{Total Heat} = \int_{-\infty}^{\infty} u(x,t)\,dx = \int_{-\infty}^{\infty} f(y)\int_{-\infty}^{\infty}\Phi(x-y,t)\,dx\,dy = \int_{-\infty}^{\infty} f(y)\,dy$$

is constant in time. Notice we exchanged the order of integration in the second step.

2. All partial derivatives of u pass through the integral and fall onto the source function. For example

$$u_{xxt}(x,t) = \int_{-\infty}^{\infty}\Phi_{xxt}(x-y,t)f(y)\,dy.$$

Since Φ is infinitely differentiable, we see that u is also infinitely differentiable for all $t > 0$. This is true regardless of whether the initial condition $f(x) = u(x,0)$ is even differentiable! Thus, the heat equation instantaneously smoothes out the initial data.



(a) Noisy signal (b) Small t

(c) Moderate t (d) Large t

Figure 3: Denoising a signal with the heat equation.

3. The heat equation supports *infinite speed of propagation*. Indeed, suppose the initial condition is
$$f(x) = \begin{cases} 1, & \text{if } -1 \leq x \leq 1 \\ 0, & \text{otherwise.} \end{cases}$$
Then the solution of the heat equation
$$u(x,t) = \int_{-1}^{1} \Phi(x-y,t)\,dy = \frac{1}{\sqrt{4k\pi t}} \int_{-1}^{1} e^{-(x-y)^2/4kt}\,dy$$
is positive for all x and $t > 0$. Hence, the initial heat energy contained in the interval $[-1, 1]$ spreads out along the entire infinite rod *instantaneously*.

The reader should contrast property 3 with the wave equation, where information propagates at a finite speed bounded by c.

Since the heat equation smoothes the initial data, we can use it to remove noise from signals. Figure 3 shows a noisy 1D signal and the result of applying the heat equation to the signal for various amounts of time. As time increases, the signal becomes smoother and more noise is removed. At the same time, important features in the signal may be removed as well (i.e., they are mistaken for noise).

Images are 2D signals, and the heat equation was one of the first PDE proposed for noise removal in the image processing community. Here, we model an image as a function $f : [0,1]^2 \to \mathbb{R}^n$, where $n = 1$ for grayscale images, and $n = 3$ for color images. The quantity $f(x)$ is the color of the pixel at location x. We apply the 2D heat equation to each image component separately (in RGB space, or more preferably YCbCr space). Figure 4(a) shows a noisy image of Vincent Hall, and Figure 4(b) shows the result of applying the heat equation to the noisy image for a short amount of time. Notice that the noise is mostly removed, but also important image features and details are blurred. This is due to the fact that the heat equation indiscriminately blurs everything without regard for whether it is noise or an important edge in the image.

Figure 4(c) shows the result of applying a nonlinear heat equation called the Perona-Malik equation to the same noisy image. The Perona-Malik equation is given by

$$u_t - \operatorname{div}\left(k(\|\nabla u\|)\nabla u\right) = 0.$$

This is a nonlinear heat equation where the thermal conductivity k depends on the norm of the gradient $\|\nabla u\|$. The function k is chosen to be a decreasing function, so that when $\|\nabla u\|$ is large, diffusion is slowed or completely stopped, and when $\|\nabla u\|$ is small, diffusion proceeds. This smoothes the image while preserving some details and sharp edges. A common choice for k is

$$k(s) = \frac{1}{1 + s^2/M},$$

where $M > 0$ is a parameter controlling how much detail you wish to preserve in the image. Notice in Figure 4(c) that most of the noise is removed, while many of the edges and fine details in the image are preserved. The Perona-Malik equation is not the only PDE used in image processing—indeed, there is a very active research field at the intersection of PDE and image processing.

(a) Noisy image

(b) Denoising with the heat equation

(c) Denoising with the Perona-Malik equation

Figure 4: Denoising an image with the heat equation. The heat equation (b) indiscriminately blurs edges and removes image detail, while the Perona-Malik equation (c) removes noise while preserving edges and some fine details.