Deriving the Heat Equation

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1 The Heat Equation in One Dimension

Let us consider the initial value problem of the heat equation,

$$\begin{cases} u_t - u_{xx} = 0 & t > 0, \quad -\infty < x < \infty \\ u(x,0) = f(x), & \quad -\infty < x < \infty \end{cases} \tag{1}$$

where the derivatives of u are continuous, and f is continuous and bounded.

First, we will symbolically derive the solution formula using the Fourier transform with respect to x. Then, we will use the theorems studied in Advanced Calculus in order to justify that this formula is indeed a solution to the heat equation and satisfies the initial condition at $t = 0$. Moreover, we will show that the solution is unique.

Deriving the Solution

To begin, we rewrite (1) under the Fourier transform with respect to x. We define the *Fourier transform* of $u(x,t)$ by

$$\hat{u}(\omega,t) \equiv \mathcal{F}[u] = \int_{-\infty}^{\infty} u(x,t)e^{i\omega x}\,dx, \tag{2}$$

and the *inverse* Fourier transform of $\hat{u}(\omega,t)$ by

$$u(x,t) \equiv \mathcal{F}^{-1}[\hat{u}] = \frac{1}{2\pi}\int_{-\infty}^{\infty} \hat{u}(\omega,t)e^{-i\omega x}\,d\omega.^{1} \tag{3}$$

[1] We sometimes use the expressions "image of–" and "preimage of–" in place of "Fourier transform of–" and "inverse Fourier transform of–", respectively.

The heat equation in (1) becomes

$$\hat{u}_t - \hat{u}_{\omega\omega} = 0. \tag{4}$$

We note that

$$\begin{aligned}
\hat{u}_{\omega\omega} &= \frac{\partial^2}{\partial\omega^2}\int_{-\infty}^{\infty} u(x,t)e^{i\omega x}\,dx \\
&= \int_{-\infty}^{\infty} u(x,t)\frac{\partial^2}{\partial\omega^2}e^{i\omega x}\,dx \\
&= (i\omega)^2\int_{-\infty}^{\infty} u(x,t)e^{i\omega x}\,dx \\
&= -\omega^2\hat{u}.
\end{aligned}$$

By substituting this result into (4), we immediately obtain the first-order differential equation,

$$\hat{u}_t + \omega^2\hat{u} = 0. \tag{5}$$

Then, we take the Fourier transform of f in (1) to obtain

$$\begin{cases} \hat{u}_t + \omega^2\hat{u} = 0 & t > 0, \quad -\infty < \omega < \infty \\ \hat{u}(\omega, 0) = \hat{f}(\omega), & -\infty < \omega < \infty \end{cases} \tag{6}$$

where $\hat{f} \equiv \mathcal{F}[f]$. The initial value problem (6) has the solution,

$$\hat{u}(\omega, t) = \hat{f}(\omega)e^{-\omega^2 t}. \tag{7}$$

We may now obtain u from $\hat{u}$ by using the convolution theorem for the Fourier transform, which states,

$$\mathcal{F}(f * g) = \hat{f}(\omega)\hat{g}(\omega), \tag{8}$$

where the convolution of f and g, denoted here by $f * g$, is defined by

$$f * g = \int_{-\infty}^{\infty} f(\xi)g(x - \xi)\,d\xi. \tag{9}$$

As defined previously, the preimage of $\hat{f}$ is f. However, we must compute the preimage of $e^{-\omega^2 t}$:

$$\begin{aligned}
\mathcal{F}^{-1}[e^{-\omega^2 t}] &= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-\omega^2 t}e^{-i\omega x}\,d\omega \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-\omega^2 t}\left[\cos(\omega x) - i\sin(\omega x)\right]\,d\omega \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-\omega^2 t}\cos(\omega x)\,d\omega - \frac{i}{2\pi}\int_{-\infty}^{\infty} e^{-\omega^2 t}\sin(\omega x)\,d\omega.
\end{aligned}$$

Since $e^{-\omega^2 t}$ and $\cos(\omega x)$ are even functions, and $\sin(\omega x)$ is an odd function, this reduces to

$$\mathcal{F}^{-1}[e^{-\omega^2 t}] = \frac{1}{\pi}\int_0^\infty e^{-\omega^2 t}\cos(\omega x)\,d\omega.$$

Evaluating the integral, we find

$$\mathcal{F}^{-1}[e^{-\omega^2 t}] = \frac{e^{-\frac{x^2}{4t}}}{\sqrt{4\pi t}}.$$

Thus, by the convolution theorem, we reach the solution

$$u(x,t) = \int_{-\infty}^{\infty} f(\xi)k(x-\xi)\,d\xi, \tag{10}$$

where

$$k(x,t) = \frac{e^{-\frac{x^2}{4t}}}{\sqrt{4\pi t}} \tag{11}$$

is called the *heat kernel*. It should be pointed out that the heat kernel itself satisfies the heat equation.

Justifying the Solution

What remains to be done is to show that (10) is indeed a solution by verifying

$$u_{xx} - u_t = \int_{-\infty}^{\infty} f(\xi)\left(\frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial t}\right)k(x-\xi)\,d\xi = 0. \tag{12}$$

Since k is a solution, clearly this is true if we can justify taking the derivatives, $\frac{\partial}{\partial x}$, $\frac{\partial^2}{\partial x^2}$, and $\frac{\partial}{\partial t}$ under the integral sign. Before doing so, we apply a change of variables, $\bar{\xi} = \xi - x$, to obtain

$$u_{xx} - u_t = \int_{-\infty}^{\infty} f(\bar{\xi}+x)\left(\frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial t}\right)k(\bar{\xi})\,d\bar{\xi} = 0, \tag{13}$$

and show the uniform convergence of each derivative in (13).

Suppose

$$|f(\bar{\xi}+x)| \le R. \qquad -\infty < x < \infty$$

Then, we have

$$\left|f(\bar{\xi}+x)\frac{\partial}{\partial x}\frac{e^{-\frac{\bar{\xi}^2}{4t}}}{\sqrt{4\pi t}}\right| = \left|f(\bar{\xi}+x)\frac{\bar{\xi}}{2t}\right|\frac{e^{-\frac{\bar{\xi}^2}{4t}}}{\sqrt{4\pi t}}$$

$$\leq \frac{R\bar{\xi}}{2t_0}\frac{e^{-\frac{\bar{\xi}^2}{4T}}}{\sqrt{4\pi t_0}} = M_1(\bar{\xi}),$$

whenever $0 < t_0 \leq t \leq T$. Since $\int_0^\infty M_1(\bar{\xi})\,d\bar{\xi}$ converges,

$$\int_{-\infty}^{\infty} f(\bar{\xi}+x)\frac{\partial}{\partial x}k(\bar{\xi},t)\,d\bar{\xi}$$

converges uniformly in $0 < t_0 \leq t \leq T$.

Again, since

$$|f(\bar{\xi}+x)| \leq R, \qquad -\infty < x < \infty$$

we have

$$\left|f(\bar{\xi}+x)\frac{\partial^2}{\partial x^2}\frac{e^{-\frac{\bar{\xi}^2}{4t}}}{\sqrt{4\pi t}}\right| = \left|f(\bar{\xi}+x)\left[\frac{\bar{\xi}}{4t^2}-\frac{1}{2t}\right]\frac{e^{-\frac{\bar{\xi}^2}{4t}}}{\sqrt{4\pi t}}\right|$$

$$= |f(\bar{\xi}+x)|\left|\frac{\bar{\xi}}{4t^2}-\frac{1}{2t}\right|\frac{e^{-\frac{\bar{\xi}^2}{4t}}}{\sqrt{4\pi t}},$$

which, by the triangle inequality,

$$\leq \left|f(\bar{\xi}+x)\frac{\bar{\xi}}{4t^2}\right|\frac{e^{-\frac{\bar{\xi}^2}{4t}}}{\sqrt{4\pi t}} + \left|f(\bar{\xi}+x)\frac{1}{2t}\right|\frac{e^{-\frac{\bar{\xi}^2}{4t}}}{\sqrt{4\pi t}}$$

$$\leq R\left|\frac{\bar{\xi}}{4t_0^2}+\frac{1}{2t_0}\right|\frac{e^{-\frac{\bar{\xi}^2}{4T}}}{\sqrt{4\pi t_0}} = M_2(\bar{\xi}),$$

whenever $0 < t_0 \leq t \leq T$. Since $\int_0^\infty M_2(\bar{\xi})\,d\bar{\xi}$ converges,

$$\int_{-\infty}^{\infty} f(\bar{\xi}+x)\frac{\partial}{\partial x}k(\bar{\xi},t)\,d\bar{\xi}$$

converges uniformly in $0 < t_0 \leq t \leq T$.

Finally, since

$$\frac{\partial^2}{\partial x^2}k(x-\xi,t) = \frac{\partial}{\partial t}k(x-\xi,t),$$

the above argument also shows the uniform convergence of the derivative with respect to t inside the integral sign.

Thus, the solution formula given in (10) satisfies the heat equation. However, to finally conclude that the solution formula is indeed a solution, we must lastly show that the solution formula satisfies the initial condition at $t = 0$. To do so, we show that as $t \to 0$, for all $x_0 \in \mathbb{R}$, the solution u approaches the initial condition, $f(x_0)$.

It suffices to show that as $t \to 0$, for all $\epsilon > 0$, there exists some $\delta > 0$ such that

$$|u(x,t) - f(x_0)| < \epsilon \tag{14}$$

whenever $x_0 \in \mathbb{R}$ and $|x - x_0| < \frac{\delta}{2}$.

Since

$$\int_{-\infty}^{\infty} k(x-\xi,t)\,d\xi = 1,$$

it follows that

$$\int_{-\infty}^{\infty} f(x_0)k(x-\xi,t)\,d\xi = f(x_0).$$

Then, we may write

$$\begin{aligned}|u(x,t) - f(x_0)| &= \left|\int_{-\infty}^{\infty} [f(\xi) - f(x_0)]\,k(x-\xi,t)\,d\xi\right|.\\ &= \left|\int_{|\xi-x_0|<\delta} [f(\xi) - f(x_0)]\,k(x-\xi,t)\,d\xi\right.\\ &\qquad \left.+ \int_{|\xi-x_0|\geq\delta} [f(\xi) - f(x_0)]\,k(x-\xi,t)\,d\xi\right|.\end{aligned}$$

The first term, by the definition of continuity, may be defined to be less than $\frac{\epsilon}{2}$. Thus, we obtain

$$|u(x,t) - f(x_0)| \leq \frac{\epsilon}{2} + \left|\int_{|\xi-x_0|\geq\delta} [f(\xi) - f(x_0)]\,k(x-\xi,t)\,d\xi\right|.$$

Now, since $[f(\xi) - f(x_0)] < 2R$. Then,

$$|u(x,t) - f(x_0)| \leq \frac{\epsilon}{2} + \left| 2R \int_{|\xi - x_0| \geq \delta} k(x-\xi, t)\, d\xi \right|.$$

We apply a change of variables, $\bar{\xi} = \xi - x$, to get

$$|u(x,t) - f(x_0)| \leq \frac{\epsilon}{2} + \left| 2R \int_{|\bar{\xi} + x - x_0| \geq \delta} \frac{e^{-\frac{\bar{\xi}^2}{4t}}}{\sqrt{4\pi t}}\, d\bar{\xi} \right|.$$

Since $|x - x_0| \leq \frac{\delta}{2}$, we find:

$$\begin{aligned} &\delta \leq \left|\bar{\xi} + x - x_0\right| \leq \left|\bar{\xi}\right| + |x - x_0| \leq \left|\bar{\xi}\right| + \frac{\delta}{2} \\ &\frac{\delta}{2} \leq \left|\bar{\xi}\right|. \end{aligned}$$

Substituting this result, we obtain

$$|u(x,t) - f(x_0)| \leq \frac{\epsilon}{2} + \left| 2R \int_{|\bar{\xi}| \geq \frac{\delta}{2}} \frac{e^{-\frac{\bar{\xi}^2}{4t}}}{\sqrt{4\pi t}}\, d\bar{\xi} \right|.$$

Next, we apply yet another change of variables, $y^2 = \frac{\bar{\xi}^2}{4t}$, to get

$$\begin{aligned} |u(x,t) - f(x_0)| &\leq \frac{\epsilon}{2} + \left| 2R \int_{|y| \geq \frac{\delta}{4\sqrt{t}}} e^{-y^2}\, dy \right| \\ &\leq \frac{\epsilon}{2} + \left| 4R \int_{\frac{\delta}{4\sqrt{t}}}^{\infty} e^{-y^2}\, dy \right|. \end{aligned}$$

Clearly, as $t \to 0$, $\frac{\delta}{4\sqrt{t}}$ will approach the neighborhood of infinity. By choosing t small enough so that

$$\left| 4R \int_{\frac{\delta}{4\sqrt{t}}}^{\infty} e^{-y^2}\, dy \right| \leq \frac{\epsilon}{2},$$

we show that

$$|u(x,t) - f(x_0)| \leq \frac{\epsilon}{2} + \frac{\epsilon}{2} \leq \epsilon.$$

This completes the proof.

Thus, we have shown that (10) is indeed a solution to the heat equation and satisfies the initial condition as $t \to 0$.

Uniqueness of the Solution

Now, we wish to show that the solution is unique. For the bounded function f, clearly
$$\inf_{x\in\mathbb{R}} f(\xi) = m \leq f(\xi) \leq M = \sup_{x\in\mathbb{R}} f(\xi).$$
It follows that
$$m\, k(x-\xi,t) \leq f(\xi)k(x-\xi,t) \leq M\, k(x-\xi,t),$$
which we integrate to obtain,
$$m\int_{-\infty}^{\infty} k(x-\xi,t)\,d\xi \leq \int_{-\infty}^{\infty} f(\xi)k(x-\xi,t)\,d\xi \leq M\int_{-\infty}^{\infty} k(x-\xi,t)\,d\xi.$$
Since $\int_{-\infty}^{\infty} k(x-\xi,t)\,d\xi = 1$, it follows that
$$\inf_{x\in\mathbb{R}} f(\xi) = m \leq u(x,t) \leq M = \sup_{x\in\mathbb{R}} f(\xi). \tag{15}$$
Suppose u_1 and u_2 are two solutions of the initial value problem,
$$\begin{cases} u_t - u_{xx} = 0 & t>0, \quad -\infty < x < \infty \\ u(x,0) = f(x). & \quad -\infty < x < \infty \end{cases}$$
Then, $u = u_1 - u_2$ satisfies the problem,
$$\begin{cases} u_t - u_{xx} = 0 & t>0, \quad -\infty < x < \infty \\ u(x,0) = f(x) = 0. & \quad -\infty < x < \infty \end{cases}$$
Therefore, using (15), we realize
$$0 \leq u(x,t) \leq 0,$$
which implies that $u = u_1 - u_2 \equiv 0$. Thus, the solution is unique.

2 The Heat Equation in Three Dimensions

In the previous section, we derived the solution to the heat equation, showed directly that it was indeed a solution and that it satisfied the initial condition, and proved its uniqueness. We now briefly generalize these notions to three spatial dimensions.

The initial value problem of the heat equation, in three dimensions, is

$$\begin{cases} u_t - \bigtriangledown^2 u = 0 & t > 0, \quad \vec{x} \in \mathbb{R}^3 \\ u(\vec{x}, 0) = f(\vec{x}), & \vec{x} \in \mathbb{R}^3 \end{cases}$$

where the derivatives of u are continuous, and f is continuous and bounded. To derive the solution, we rewrite the problem under the three dimensional Fourier transform:

$$\begin{cases} \hat{u}_t - ||\vec{\omega}||^2 \hat{u} = 0 & t > 0, \quad \vec{\omega} \in \mathbb{R}^3 \\ \hat{u}(\vec{\omega}, 0) = \hat{f}(\vec{\omega}). & \vec{\omega} \in \mathbb{R}^3 \end{cases}$$

This initial value problem has the solution,

$$\hat{u}(\vec{\omega}, t) = \hat{f}(\vec{\omega}) e^{-||\vec{\omega}||^2 t}.$$

As with the one-dimensional solution, we obtain u from $\hat{u}$ by using the convolution theorem for the Fourier transform:

$$u(\vec{x}, t) = \int \int \int_{-\infty}^{\infty} f(\vec{\xi}) k(\vec{x} - \vec{\xi}) \, d\xi_1 d\xi_2 d\xi_3,$$

where

$$k(\vec{x}, t) = \frac{e^{-\frac{||\vec{x}||^2}{4t}}}{(4\pi t)^{3/2}}$$

is the new heat kernel.

From hereon, the steps for justifying the solution, showing satisfaction of the initial condition, and even showing uniqueness are analogous to that of the one-dimensional solution. Concepts such as uniform convergence, continuity, and the theorems revolving around them are carried into higher dimensions.