Diffusion equation in one spatial variable – Cauchy problem.

$$u_t(x,t) - k\,u_{xx}(x,t) = f(x,t), \quad x \in \mathbb{R},\ t > 0$$

$$u(x,0) = \varphi(x)$$

Some more mathematics

$$\Theta(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x > 0 \end{cases}$$

is the *Heaviside* step function.

It holds

$$\Theta'(x) = \delta(x)$$

where δ is the *Dirac delta function.*

Some *properties* of delta function:

Intuitively,

$$\delta(x) \; = \; \begin{cases} 0 & \text{if } x \neq 0 \\ \infty & \text{if } x = 0 \end{cases}$$

For any continuous function f, it holds

$$\int_{-\infty}^{\infty} \delta(y) f(y) dy \; = \; f(0)$$

The latter relation implies

$$\int_{-\infty}^{\infty} \delta(x-y)\varphi(y)dy \;=\; \varphi(x)$$

for any continuous function φ.

The integral $\int_{-\infty}^{\infty} g(x-y)f(y)dy$ is called the *convolution* of functions g and f.

The transformation of the step function Θ to an arbitary continuous function φ:

$$\Theta \quad \underset{\text{differentiation}}{\longrightarrow} \quad \delta \quad \underset{\text{convolution}}{\longrightarrow} \quad \varphi$$

Cauchy problem for homogeneous equation with step function

$$w_t(x,t) - k\,w_{xx}(x,t) = 0, \quad x \in \mathbb{R},\ t > 0$$
$$w(x,0) = \Theta(x)$$

We transform the equation

$$w_t(x,t) - k\,w_{xx}(x,t) = 0$$

to an ordinary differential equation by means of the change of variables

$$w(x,t) = f(z)\,, \quad z = \frac{x}{\sqrt{4kt}}$$

Compute:

$$w_t = f'(z) z_t = -\frac{1}{2} \frac{x}{\sqrt{4kt^3}} f'(z)$$

$$w_x = f'(z) z_x = \frac{1}{\sqrt{4kt}} f'(z)$$

$$w_{xx} = \frac{\partial}{\partial x} w_x = \frac{1}{4kt} f''(z)$$

Substituting these formulas to the equation $w_t(x,t) - k\, w_{xx}(x,t) = 0$ we deduce

$$0 = w_t - k w_{xx} = -\frac{1}{2} \frac{x}{\sqrt{4kt^3}} f'(z) - k \frac{1}{4kt} f''(z) = -\frac{1}{4t} f''(z) - \frac{1}{2} \frac{x}{\sqrt{4kt^3}} f'(z) =$$

$$= -\frac{1}{4t} \left[f''(z) + \frac{4tx}{2\sqrt{4kt^3}} f'(z) \right] = -\frac{1}{4t} \left[f''(z) + \frac{2x}{\sqrt{4kt}} f'(z) \right] = -\frac{1}{4t} [f''(z) + 2z f'(z)].$$

Thus, we obtain the ordinary ordinary differential equation

$$f''(z) + 2z f'(z) = 0. \qquad (*)$$

Denote $g = f'$. Then the equation is $g'(z) + 2zg(z) = 0$. We solve it:

$$\frac{dg}{dz} = -2zg \;\Rightarrow\; \frac{dg}{g} = -2z dz \;\Rightarrow\; \int \frac{dg}{g} = -\int 2z dz \;\Rightarrow\; \ln |g| = -z^2 + c_1 \;\Rightarrow\; g = c_1 e^{-z^2}$$

Further,

$$f' = c_1 e^{-z^2} \;\Rightarrow\; f(z) = c_1 \int_0^z e^{-s^2} ds + c_2$$

The general solution of the equation (*) is

$$f(z) = c_1 \int_0^z e^{-s^2} ds + c_2$$

where c_1, c_2 are arbitrary constants.

Consequently,

$$w(x,t) = c_1 \int_0^{\frac{x}{\sqrt{4kt}}} e^{-s^2} ds + c_2$$

We use the initial condition $w(x,0) = \Theta(x)$ to determine the constants c_1 and c_2.

In case $x < 0$ and $t \to 0^+$

$$0 = w(x,0) = c_1 \int_0^{-\infty} e^{-s^2} ds + c_2 = -c_1 \int_0^{\infty} e^{-s^2} ds + c_2$$

In case $x > 0$ and $t \to 0^+$

$$1 = w(x,0) = c_1 \int_0^{\infty} e^{-s^2} ds + c_2$$

It is known that $\int_0^\infty e^{-s^2} ds = \frac{\sqrt{\pi}}{2}$. Therefore,

$$\begin{cases} -\frac{\sqrt{\pi}}{2}\, c_1 + c_2 = 0 \\ \frac{\sqrt{\pi}}{2}\, c_1 + c_2 = 1 \end{cases}$$

Solving this linear system we get $c_1 = \frac{1}{\sqrt{\pi}}$, $c_2 = \frac{1}{2}$.

The solution of the posed Cauchy problem with step function is

$$w(x,t) = \frac{1}{2} + \frac{1}{\sqrt{\pi}} \int_0^{\frac{x}{\sqrt{4kt}}} e^{-s^2} ds$$

Using the *error function* $\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-s^2} ds$
the solution is written in the form

$$w(x,t) = \frac{1}{2}\left[1 + \operatorname{erf}\left(\frac{x}{\sqrt{4kt}}\right)\right]$$

This not a classical solution (w is not continuous).

Cauchy problem for homogeneous equation with delta function

$$G_t(x,t) - k\,G_{xx}(x,t) = 0, \quad x \in \mathbb{R},\ t > 0$$

$$G(x,0) = \delta(x)$$

The previous problem was

$$w_t(x,t) - k\,w_{xx}(x,t) = 0, \quad x \in \mathbb{R},\ t > 0$$

$$w(x,0) = \Theta(x)$$

Since $\Theta' = \delta$, it holds $G = w_x$.

From the formula

$$w(x,t) = \frac{1}{2} + \frac{1}{\sqrt{\pi}} \int_0^{\frac{x}{\sqrt{4kt}}} e^{-s^2} ds$$

we obtain the formula for G:

$$G(x,t) = w_x(x,t) = \frac{1}{\sqrt{4\pi kt}}\, e^{-\frac{x^2}{4kt}}$$

G is called the heat (diffusion) kernel or the fundamental solution of the diffusion equation.

Cauchy problem for homogeneous equation in general case

$$u_t(x,t) - k\, u_{xx}(x,t) = 0, \quad x \in \mathbb{R},\ t > 0$$
$$u(x,0) = \varphi(x)$$

where φ is an arbitrary given function.

Due to the properties of the delta function,

$$\int_{-\infty}^{\infty} G(x-y,t)\varphi(y)dy\bigg|_{t=0} = \int_{-\infty}^{\infty} G(x-y,0)\varphi(y)dy =$$
$$= \int_{-\infty}^{\infty} \delta(x-y)\varphi(y)dy = \varphi(x)$$

This suggests that

$$u(x,t) = \int_{-\infty}^{\infty} G(x-y,t)\varphi(y)dy$$

Verification of the equation:

We obtain

$$\left(\frac{\partial}{\partial t} - k\,\frac{\partial^2}{\partial x^2}\right)\int_{-\infty}^{\infty} G(x-y,t)\varphi(y)dy = \int_{-\infty}^{\infty}\left(\frac{\partial}{\partial t} - k\,\frac{\partial^2}{\partial x^2}\right) G(x-y,t)\varphi(y)dy = 0$$

because $\left(\frac{\partial}{\partial t} - k\,\frac{\partial^2}{\partial x^2}\right) G(x,t) = 0.$

Thus, indeed the solution of the Cauchy problem is

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

Theorem. Let φ be a bounded continuous function on $\mathbb{R}$. The Cauchy problem

$$u_t(x,t) - k\, u_{xx}(x,t) = 0, \quad x \in \mathbb{R},\ t > 0$$

$$u(x,0) = \varphi(x)$$

has a classical solution given by the formula

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

Cauchy problem for nonhomogeneous equation

Theorem. Let $f = f(x,t)$ and $\varphi = \varphi(x)$ be bounded and continuous functions. The Cauchy problem for the nonhomogeneous diffusion equation

$$u_t(x,t) - k\,u_{xx}(x,t) = f(x,t), \quad x \in \mathbb{R},\ t > 0$$
$$u(x,0) = \varphi(x)$$

has a classical solution given by the formula

$$u(x,t) = \int_{-\infty}^{\infty} G(x-y,t)\varphi(y)dy + \int_0^t \int_{-\infty}^{\infty} G(x-y,t-s)f(y,s)dyds \tag{1}$$

where G is the diffusion kernel.

Derivation of the formula (1) by means of the operator method.

Firstly, we solve the following Cauchy problem for ordinary differential equation:

$$\frac{d}{dt}v(t) + Av(t) = f(t),\, t > 0, \quad v(0) = \varphi \qquad (2)$$

where A and φ are given numbers.

The homogeneous equation is

$$\frac{d}{dt}v_H(t) + Av_H(t) = 0$$

The characteristic equation $\lambda + A = 0$ has the solution $\lambda = -A$.

The general solution of the homogeneous equation is

$$v_H(t) = Ce^{-At}$$

We use the variation of constants to derive a particular solution of the inhomogeneous equation

$$v_P(t) = D(t)e^{-At}$$

Putting it to the equation we get

$$D'e^{-At} - DAe^{-At} + AD(t)e^{-At} = f$$

Thus,

$$D'(t) = e^{At}f(t)$$

Consequently,

$$D(t) = \int_0^t e^{As} f(s) ds$$

and

$$v_P(t) = D(t)e^{-At} = e^{-At} \int_0^t e^{As} f(s) ds = \int_0^t e^{-A(t-s)} f(s) ds$$

The general solution of the ODE is

$$v(t) = v_H(t) + v_P(t) = Ce^{-At} + \int_0^t e^{-A(t-s)} f(s) ds$$

We find $v(0) = C$ and by initial condition $v(0) = \varphi$ we have $C = \varphi$. Thus,

$$v(t) = \varphi e^{-At} + \int_0^t e^{-A(t-s)} f(s) ds$$

We have shown that the solution of (2) is

$$v(t) \;=\; S(t)\varphi + \int_0^t S(t-s) f(s) ds$$

where

$$S(t) = e^{-tA}$$

In the particular case $f \equiv 0$, the solution of (2) is

$$v(t) = S(t)\varphi$$

We compare it with the formula of the solution of the homogeneous Cauchy problem for the diffusion equation:

$$u(x,t) = \mathcal{S}(t)\varphi \, = \int_{-\infty}^{\infty} G(x-y,t)\varphi(y)dy$$

It holds

$$\int_0^t \mathcal{S}(t-s)f(x,s)ds = \int_0^t \int_{-\infty}^{\infty} G(x-y,t-s)f(y,s)dyds$$

Using the analogy with the solution of the Cauchy problem (2) for ODE, we put together the solution of the nonhomogeneous Cauchy problem for the diffusion equation:

$$u(x,t) = \mathcal{S}(t)\varphi + \int_0^t \mathcal{S}(t-s)f(x,s)ds =$$

$$= \int_{-\infty}^{\infty} G(x-y,t)\varphi(y)dy + \int_0^t \int_{-\infty}^{\infty} G(x-y,t-s)f(y,s)dyds$$

The formula (1) is derived.

The operator $\mathcal{S}(t)$ is called the semigroup generated by the operator $A = -k\frac{\partial^2}{\partial x^2}$.

Sometimes it is written

$$\mathcal{S}(t) = e^{-tA} = e^{tk\frac{\partial^2}{\partial x^2}}$$