THE ONE-DIMENSIONAL HEAT EQUATION.

1. **Derivation.** Imagine a dilute material species free to diffuse along one dimension; a gas in a cylindrical cavity, for example. To model this mathematically, we consider the *concentration* of the given species as a function of the linear dimension and time: u(x,t), defined so that the total amount Q of diffusing material contained in a given interval [a,b] is equal to (or at least proportional to) the integral of u:

$$Q[a,b](t) = \int_{a}^{b} u(x,t)dx.$$

Then the conservation law of the species in question says the rate of change of Q[a,b] in time equals the net amount of the species flowing into [a,b] through its boundary points; that is, there exists a function d(x,t), the 'diffusion rate from right to left', so that:

$$\frac{dQ[a,b]}{dt} = d(b,t) - d(a,t).$$

It is an experimental fact about diffusion phenomena (which can be understood in terms of collisions of large numbers of particles) that the diffusion rate at any point is proportional to the gradient of concentration, with the right-to-left flow rate being positive if the concentration is *increasing* from left to right at (x,t), that is: d(x,t) > 0 when $u_x(x,t) > 0$. So as a first approximation, it is natural to set:

$$d(x,t) = ku_x(x,t), k > 0$$
 ('Fick's law of diffusion').

Combining these two assumptions we have, for any bounded interval [a, b]:

$$\frac{d}{dt} \int_a^b u(x,t)dx = k(u_x(b,t) - u_x(a,t)).$$

Since b is arbitrary, differentiating both sides as a function of b we find:

$$u_t(x,t) = ku_{xx}(x,t)$$
.

the diffusion (or heat) equation in one dimension.

(In the case of heat we take u(x,t) to be the temperature, and assume there is a function c(x) > 0 throughout the conducting medium so that the thermal energy dQ added to the system by a 'lump' of material of mass $\rho(x)dx$ (where $\rho(x)$ is the mass density) at temperature u(x,t) is $dQ = c(x)\rho(x)u(x,t)dx$. Taking c,ρ to be constant, we are back in the earlier situation.)

We'll consider four types of problems for the heat equation:

- (i) The Cauchy problem for the equation on the whole real line, where the initial temperature (or concentration) $u_0(x)$ is given and we seek u(x,t), the solution giving its evolution in time;
- (ii) Boundary-value problems on the half-line x > 0, where we assume either the temperature is held constant at x = 0 (so heat flows in or out of the system at the origin), or that there is no diffusion of heat at x = 0 (so $u_x = 0$ at the origin.)
- (iii) Boundary-value problems on a bounded interval [0, L], or periodic boundary conditions on [-L, L].
- (iv) Non-homogeneous problems, corresponding to a heat source inside the conducting material: $u_t ku_{xx} = f(x,t)$, on the whole line or on an interval.

Basic observations: (i) The time-independent solutions of the heat equation are linear functions, u = Ax + B. By subtracting an appropriate linear function, for the boundary condition where u is held constant at the endpoints we can always assume the constants are zero (Dirichlet BC).

For Neumann-type boundary conditions $u_x = 0$, or periodic, the constants are always solutions.

(iii) In general we expect the equation to gradually 'smoothe out' any oscillations in u_0 and drive it towards the simplest time-independent solution consitent with the boundary conditions (linear, or a constant.) If the limit as $t \to \infty$ is a constant, it has to be zero for Dirichlet BC, and the average value of the initial data u_0 , for Neumann or periodic BC on a bounded interval. The reason is that the integral of u over the whole interval (and therefore its average value) is constant in time (under these BC):

$$\frac{d}{dt} \int_0^L u(x,t) dx = \int_0^L u_t(x,t) dx = k \int_0^L u_{xx}(x,t) dx = k(u_x(L,t) - u_x(0,t)) = 0,$$

under Neumann BC, and similarly under periodic BC.

(iv) Scaling. The change of variables $t \mapsto s = kt, x \mapsto x$ changes the equation $u_t = ku_{xx}$ to $u_s = u_{xx}$; the change of variables $t \mapsto t, x \mapsto y = \sqrt{kx}$ changes it to $u_t = u_{yy}$. The simultaneous change $t \mapsto s = \lambda t, x \mapsto y = \sqrt{\lambda}x$ (with $\lambda > 0$) leads back to the original equation: $u_s = ku_{yy}$ (verify these

statments). Thus we see that "one time dimension corresponds to two space dimensions", in the sense that any scaling of the variables that doesn't change the ratio x/\sqrt{t} also leaves the equation unchanged.

We also see that one can always assume the constant k equals one, by rescaling the time variable. We will usually do that, and the correct expressions for the equation with general k>0 can be recovered simply by making the change $t\to kt$.

2. The heat kernel on the real line.

2.1 Derivation. To look for exact solutions of $u_t = u_{xx}$ on \mathbb{R} (for t > 0), we remember the scaling fact just observed and try to find solutions of the form:

$$u(x,t) = p(\frac{x}{\sqrt{t}}), \quad p = p(y).$$

The heat equation quickly leads to the ODE for p(y):

$$p''(y) = -\frac{y}{2}p'(y),$$

and setting q(y) = p'(y), we find a first-order linear ODE with an easily derived general solution:

$$q'(y) = -\frac{y}{2}q(y) \longrightarrow q(y) = Ce^{-y^2/4}, C > 0, y \in \mathbb{R}.$$

Thus the function P(x,t) below is a solution of the heat equation on the real line:

$$P(x,t) = \int_0^{x/\sqrt{T}} e^{-^2/4} dy = \frac{1}{2} \int_0^{x/\sqrt{4t}} e^{-p^2} dp.$$

Now recall the well-known fact from Calculus:

$$\int_{0}^{\infty} e^{-p^2} dp = \frac{\sqrt{\pi}}{2}$$

and the related definition of the "Error Function":

$$ERF(z) = \frac{1}{2} + \frac{1}{\sqrt{\pi}} \int_0^z e^{-p^2} dp, z \in \mathbb{R}.$$

This function has the properties:

 $\lim_{z\to -\infty} ERF(z) = 0, \lim_{z\to \infty} ERF(z) = 1, ERF(0) = \frac{1}{2}, ERF(z) - \frac{1}{2} \text{ is an odd function of } z.$

And so instead of using P(x,t) we define:

$$H(x,t) = ERF(\frac{x}{\sqrt{4t}}),$$

a solution of the heat equation $u_t - u_{xx} = 0$. The normalization constants are chosen so that the limit of this solution as $t \to 0_+$ is (pointwise in x) the (discontinuous!) function $\theta(x)$ defined by:

$$\theta(x) = 0, x < 0; \theta(0) = ERF(0) = \frac{1}{2}, \theta(x) = 1, x > 0.$$

(Engineers will recognize this as "Heaviside's unit step function at zero".)

Unfortunately we only found an exact solution of the heat equation given as an integral, so just in case we check whether $u(x,t) = exp(-x^2/4t)$ is a solution of $u_t = u_{xx}$ and find that it is *not*. Computing its integral over the whole real line, we find (*check!*):

$$\int_{-\infty}^{\infty} e^{-\frac{x^2}{4t}} dx = \sqrt{4\pi t}.$$

This moves us to consider the function:

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

and it turns out this one works (and is called the *heat kernel* on the real line):

Exercise: Show that h(x,t) is a solution of $u_t = u_{xx}$ for $x \in \mathbb{R}, t > 0$, and satisfies: $\int_{-\infty}^{\infty} h(x,t)dx = 1$.

2.2 Relation with the normal distribution. To understand the behavior of h(x,t), we note that its graph is an even "bell-shaped curve" centered at 0 and with "thickness" of the peak apparently related to t (sharper peak, the smaller t>0 is.) Recall the "standard normal probability density function" from Probability:

$$p(x;0,1) = \frac{1}{\sqrt{2\pi}}e^{-\frac{x^2}{2}},$$

as well as the more general "normal probability density function with mean value $\mu \in \mathbb{R}$ and standard deviation $\sigma > 0$ ":

$$p(x; \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{(x-\mu)^2}{2\sigma^2}}.$$

Its graph is the "bell-shaped curve" with peak value at $x = \mu$ and peak width proportional to σ . Its integral over the whole real line is one, for all $\mu \in \mathbb{R}, \sigma > 0$.

If you've studied some probability (and you should), you'll recall that for a normally distributed random variable X taking values on \mathbb{R} , with expected value (mean) μ and standard deviation σ (or *variance* σ^2), we have the probabilities:

$$Pr_{\mu,\sigma}[a \le X \le b] = \int_a^b p(x;\mu,\sigma)dx.$$

The cumulative distribution function for p(x; 0, 1) is exactly ERF!

$$Pr_{0,1}[X \le z] = \int_{-\infty}^{z} p(x; 0, 1) dx = ERF(z),$$

and with mean μ and standard deviation σ :

$$Pr_{\mu,\sigma}[X \le x] = \int_{-\infty}^{x} p(y;\mu,\sigma)dy = ERF(\frac{x-\mu}{\sigma\sqrt{2}}).$$

The connection with the heat equation then is: we have the correspondence $\sigma^2 \leftrightarrow 2t$ (time corresponds to variance). For the heat kernel and normal probability density function.:

$$p(x; 0, 1) = h(x, \frac{1}{2}); \quad p(x; \mu, \sigma) = h(x - \mu, \frac{\sigma^2}{2}).$$

For the integrated solution H(x,t) and normal cumulative distribution function:

$$ERF(z) = H(z, \frac{1}{2}); \quad ERF(\frac{x-\mu}{\sigma\sqrt{2}}) = H(x-\mu, \frac{\sigma^2}{2}).$$

2.3 Solutions for step-function initial data.

It is easy to use linearity and the 'translation invariance' (u(x-a,t)) is a solution of the heat equation if u(x,t) is) to write down the solutions of $u_t = u_{xx}$ with for simple discontinuous initial data. For example, consider the function:

$$\theta_{a,b}(x) = 0, x < a, \theta_{a,b}(x) = 1, a < x < b, \theta_{a,b}(x) = 0, x > b, \theta_{a,b}(a) = \theta_{a,b}(b) = \frac{1}{2}$$

Then $\theta_{a,b}(x) = \theta_a(x) - \theta_b(x)$, where $\theta_a(x) = \theta(x-a)$ is the Heaviside unit step function with jump discontinuity at x = a. It is easy to see that:

$$H_{a,b}(x,t) = H(x-a,t) - H(x-b,t) = ERF(\frac{x-a}{\sqrt{4t}}) - ERF(\frac{x-b}{\sqrt{4t}})$$

is a solution of $u_t - u_{xx} = 0$ on the real line, converging pointwise to $\theta_{a,b}(x)$ as $t \to 0_+$. This generalizes to arbitrary 'step functions': take a partition $a_1 \le a_2 \le \ldots \le a_N \le a_{N+1}$ of the interval $[a_1, a_{N+1}]$ into N adjacent sub-intervals, and given real constants c_1, \ldots, c_N define:

$$u_0(x) = \sum_{i=1}^{N} c_i \theta_{a_i, a_{i+1}}(x).$$

This is a piecewise-constant function with jump discontinuities at the a_i , and vanishing outside $[a_1, a_{N+1}]$. The solution of the heat equation with this initial function is simply:

$$u(x,t) = \sum_{i=1}^{N} c_i H_{a_i,a_{i+1}}(x,t) = \sum_{i=1}^{N} c_i (ERF(\frac{x-a_i}{\sqrt{4t}}) - ERF(\frac{x-a_{i+1}}{\sqrt{4t}})).$$

Exercise: Show that for each $i=2,\ldots,N$, we have: $\lim_{t\to 0_+} u(a_i,t)=\frac{c_{i-1}+c_i}{2}$.

3. Solution of the Cauchy problem.

We first recall some basic definitions in Analysis. Let $f: I \to \mathbb{R}$ be a function, where $I \subset \mathbb{R}$ is an open interval.

Definition. Let $x \in I$. f is continuous at $x \in I$ if:

$$(\forall \epsilon > 0)(\exists \delta > 0)(|x - y| < \delta, y \in I \Rightarrow |f(x) - f(y)| < \epsilon).$$

Note that, in general, δ depends both on ϵ and on x.

f is uniformly continuous on I if:

$$(\forall \epsilon > 0)(\exists \delta > 0)(\forall x, y \in I)(|x - y| < \delta \Rightarrow |f(x) - f(y)| < \epsilon).$$

In contrast, in this case δ depends only on ϵ ; the same δ works for all x and y.

It follows from the Mean Value Theorem that if f' is continuous and bounded in I, then f is uniformly continuous on I. (If you've studied some Analysis, you can easily verify this.)

We say $f(x,t) \to f_0(x)$ pointwise on I as $t \to 0_+$ if, for each $x \in I$, we have $\lim_{t\to 0_+} f(x,t) = f_0(x)$. This means:

$$(\forall x \in I)(\forall \epsilon > 0)(\exists \tau > 0)(0 < t < \tau \Rightarrow |f(x, t) - f_0(x)| < \epsilon).$$

Here τ in general depends both on ϵ and on x.

We say $f(x,t) \to f_0(x)$ uniformly on I if $\lim_{t\to 0_+} ||f(x,t) - f_0(x)|| = 0$, where we use the 'sup norm' for bounded functions on I (that is, ||g|| is the smallest positive M so that $|g(x)| \leq M$ for all $x \in I$.) Equivalently, uniform convergence means:

$$(\forall \epsilon > 0)(\exists \tau > 0)(0 < t < \tau \Rightarrow (\forall x \in I)(|f(x,t) - f_0(x)| < \epsilon)).$$

Here τ depends on ϵ , but not on the point x in I.

Theorem. Let u_0 be a continuous, bounded function on \mathbb{R} . Denoting by h(x,t) the heat kernel on \mathbb{R} , consider the function u defined by an improper integral:

$$u(x,t) = \int_{-\infty}^{\infty} h(x-y,t)u_0(y)dy.$$

We have:

- (i) If u_0 is continuous at $x \in \mathbb{R}$, then $u(x,t) \to u_0(x)$ as $t \to 0_+$ (pointwise convergence.)
- (ii) If u_0 is uniformly continuous on \mathbb{R} , then $u(x,t) \to u_0(x)$ as $t \to 0_+$, uniformly on \mathbb{R} .
 - (iii) We have, for each $x \in \mathbb{R}$:

$$u_x(x,t) = \int_{-\infty}^{\infty} h_x(x-y,t)u_0(y)dy.$$

The same holds for u_{xx} and u_t . Since $h_t(x-y,t) = h_{xx}(x-y,t)$ for each y,t, it follows that $u_t = u_{xx}$, so u is a solution of the heat equation.

(iv) The function $(x,t) \mapsto u(x,t)$ is *smooth* in $\mathbb{R} \times \mathbb{R}_+$ (that is, has continuous partial drivatives of all orders in x and t, for any (x,t) with t > 0), even if u_0 is just continuous.

Important Remark. Part (iv) is saying that even if the graph of u_0 is "jagged" (non-differentiable)—in fact even if it has jump discontinuities, though we won't prove this—the graph of $u(\cdot,t)$ is smooth for any t>0. This instantaneous smoothing property is in stark contrast to what we observed for the WE, which propagates the singularities of the initial data for all time (alng characteristic lines.)

Corollary. Suppose there exist constants $M, N \in \mathbb{R}$ so that, for all $x \in \mathbb{R}$, we have $N \leq u_0(x) \leq M$. Then the same inequalities hold at any time t > 0:

$$N \le u(x,t) \le M$$
, for all $t > 0$.

Proof. Just note that, since the heat kernel integrates to one over the whole real line, we have:

$$u(x,t) - N = \int_{-\infty}^{\infty} h(x-y,t)(u_0(y) - N)dy,$$

and this must be greater than or equal to zero, since h(x - y, t) > 0 and $u_0(y) - N \ge 0$. the other inequality is proved in the same way. In particular, we have the *stability estimate* for the 'sup norm':

$$||u(\cdot,t)|| \le ||u_0||,$$

for each t > 0.

Convergence of improper integrals. The theorem deals with improper integrals depending on a parameter, of the type:

$$\int_{-\infty}^{\infty} f(x,t,y)dy, f: R \times \mathbb{R} \to \mathbb{R} \text{ smooth }, (x,t) \in R \subset \mathbb{R} \times \mathbb{R}_+, \text{ a rectangle.}$$

We recall some definitions and theorems used in the proof. An improper integral of this type converges absolutely for a given $(x,t) \in R$ if:

$$\lim_{A,B\to\infty} [\int_{-B}^{-A} |f(x,t,y)| dy + \int_{A}^{B} |f(x,t,y)| dy] = 0,$$

or equivalently if, at the given (x, t):

$$(\forall \epsilon > 0)(\exists A > 0)(\forall B > A) \int_{-B}^{-A} |f(x, t, y)| dy + \int_{A}^{B} |f(x, t, y)| dy < \epsilon.$$

Here A depends on ϵ , and in general also on the point (x,t). (The adjective 'absolutely' refers to the absolute value, so it is automatic if the integrand is positive.) On the other hand, we say the integral converges absolutely and uniformly in R if:

$$(\forall \epsilon > 0)(\exists A > 0)(\forall B > A)(\forall (x, t) \in R) \int_{-R}^{-A} |f(x, t, y)| dy + \int_{A}^{B} |f(x, t, y)| dy < \epsilon.$$

That is, in this case the same A works for all $(x,t) \in R$: how far out we have to take the 'tail' parts of the graph of $y \mapsto f(x,t,y)$ to be ϵ -close to the value of the integral depends only on ϵ , not on (x,t).

It is a theorem of Analysis that if f(x,t,y) and $f_x(x,t,y)$ are continuous in $R \times \mathbb{R}$, and if the improper integrals $\int_{-\infty}^{\infty} f(x,t,y) dx$ and $\int_{-\infty}^{\infty} f_x(x,t,y) dx$ converges absolutely and uniformly in R, then the function in R taking (x,t) to $\int_{-\infty}^{\infty} f(x,t,y) dx$ is continuously differentiable in R, and:

$$\frac{\partial}{\partial x} \int_{-\infty}^{\infty} f(x, t, y) dx = \int_{-\infty}^{\infty} f_x(x, t, y) dx.$$

Proof of Theorem. For (i) and (ii), given $\epsilon > 0$ (and also $x \in \mathbb{R}$ in case (i)) we must find $\tau > 0$ so that $|u(x,t) - u_0(x)| < \epsilon$ if $0 < t < \tau$, where τ may depend on x in case (i), but depends only on ϵ in case (ii). Choose $\delta > 0$ so that $|u_0(x+z) - u_0(x)| < \epsilon/2$ if $|z| < \delta$. Note δ depends on x and ϵ in case (i), but only on ϵ if u_0 is uniformly continuous (case (ii)). Now split the integral defining u(x,t) into two parts (with the change of variable $y \to z = y - x$, using also that h(x,t) is even in x):

$$u(x,t) - u_0(x) = \int_{-\infty}^{\infty} h(x-y,t)[u_0(y) - u_0(x)]dy = \int_{-\infty}^{\infty} h(z,t)(u_0(x+z) - u_0(x))dz$$
$$= (\int_{|z| > \delta} + \int_{-\delta}^{\delta} h(z,t)(u_0(x+z) - u_0(x))dz = A + B,$$

and from the choice of δ the second integral may be estimated by:

$$|B| \le \frac{\epsilon}{2} \int_{-\delta}^{\delta} h(z,t) dz < \frac{\epsilon}{2} \text{ for any } t > 0,$$

since $\int_{-\infty}^{\infty} h(z,t)dz = 1$ (and h(z,t) > 0 for all z,t). To estimate the integral A, observe that:

$$\int_{|z|>\delta} h(z,t)dz = \frac{1}{\sqrt{4\pi t}} \int_{|z|>\delta} e^{-z^2/4t} dz$$
$$= \frac{1}{\sqrt{\pi}} \int_{|y|>\frac{\delta}{\sqrt{4t}}} e^{-y^2} dy = 2(1 - ERF(\frac{\delta}{\sqrt{4t}}))$$

(the reader should verify the last equality), so that:

$$|A| \le 4||u_0||(1 - ERF(\frac{\delta}{\sqrt{4t}})),$$

and this will be smaller than $\epsilon/2$ for any $0 < t < \tau$, provided we choose τ so that:

$$(1 - ERF(\frac{\delta}{\sqrt{4\tau}})) = \frac{\epsilon}{8||u_0||}.$$

(This is possible since $\lim_{z\to\infty} ERF(z)=1$.) We see that τ depends only on $\epsilon, ||u_0||$ and δ (hence on $||u_0||$ and ϵ in case (ii), and additionally on x in case (i).)

This concludes the proofs of parts (i) and (ii) of the Theorem. To prove part (iii) using the differentiability criterion recalled above, we just have to show that the integral:

$$\int_{-\infty}^{\infty} |h_x(x-y,t)u_0(y)| dy = \frac{1}{2t\sqrt{4\pi t}} \int_{-\infty}^{\infty} |x-y| e^{-(x-y)^2/4t} |u_0(y)| dy$$

is uniformly convergent for $(x,t) \in \mathbb{R} \times [\tau,\infty)$, for any $\tau > 0$. Making the change of variable $y \to z = (y-x)/\sqrt{4t}$, this equals:

$$\frac{1}{2t\sqrt{\pi}} \int_{-\infty}^{\infty} |z| e^{-z^2} |u_0(x+z\sqrt{4t})| dz < \frac{||u_0||}{2\tau\sqrt{\pi}} \int_{-\infty}^{\infty} |z| e^{-z^2} dz$$

for $t > \tau$. Now, since $\int_{-\infty}^{\infty} |z| e^{-z^2} dz$ is convergent, given $\epsilon > 0$ we may choose A > 0 (depending on τ and $||u_0||$) so that, for any B > A:

$$\left(\int_{-B}^{-A} + \int_{A}^{B}\right) |z| e^{-z^{2}} dz < 2\tau \sqrt{\pi} ||u_{0}||^{-1} \epsilon,$$

and then the sum of the 'tail ends' of the previous integral (defined by limits of integration z=-A,-B and z=A,B) will be smaller than ϵ , for any $x\in\mathbb{R}$ and any $t>\tau$. This concludes the proof of uniform convergence of the integral. The proofs for u_{xx} and u_t follow the same model, using the convergence of the integral

$$\int_{-\infty}^{\infty} z^2 e^{-z^2} dz.$$

This concludes the proof of part (iii) of the theorem.

For part (iv), the argument showing existence and continuity of higherorder partial derivatives of u(x,t) in the open half-plane $\{(x,t); t>0\}$ is completely analogous. For instance, showing the existence and continuity of the partial derivative of order k in x involves (in the same way as above) the convergence of the improper integral:

$$\int_{-\infty}^{\infty} |z|^k e^{-z^2} dz.$$

4. The Maximum Principle.

It is physically reasonable that, since temperature tends to become more uniform under the usual boundary conditions, the maximum and minimum temperatures sould be attained either at time zero or on the boundary. This is reflected in an important property of solutions of the heat equation, the maximum principle. At the most basic level, it is a consequence of the "second derivative test" for functions of two variables. In the following by upper half plane we mean the set $\{(x,t); x \in \mathbb{R}, t \geq 0\}$.

Calculus maximum principle. A solution of the heat equation cannot have a nondegenerate local maximum or minimum in any open region of the upper half-plane.

Proof. At a nondegenerate local max (resp. min) we have $u_t = 0$ and $u_{xx} < 0$ (resp. $u_{xx} > 0$), and this is incompatible with the equation $u_t = ku_{xx}$.

Let $R = [a, b] \times [0, T]$ be a rectangle in the upper half-plane. The *parabolic* boundary of R is the usual boundary of R, except for the top edge:

$$\partial_n R = [a, b] \times \{0\} \cup \{a, b\} \times [0, T].$$

Maximum principle. Let u(x,t) be a solution of the heat equation $u_t = ku_{xx}$ in a rectangle $[0, L] \times [0, T]$ in the upper half-plane. Then the maximum and the minimum values of u in R are attained on the parabolic boundary $\partial_p R$. In other words:

$$\max_{(x,t)\in R}u(x,t)=\max_{(x,t)\in\partial_pR}u(x,t),\quad \min_{(x,t)\in R}u(x,t)=\min_{(x,t)\in\partial_pR}u(x,t).$$

Proof. Let C > 0 be arbitrary, and define $v(x,t) = u(x,t) + Cx^2$. Then v satisfies in R:

$$v_t - kv_{xx} = u_t - ku_{xx} - 2kC = -2kC < 0.$$

Thus the maximum value of v in R cannot be attained at an interior point of R (at such an interior max, we'd have $v_t = 0, v_{xx} \le 0$, hence $v_t - kv_{xx} \ge 0$). Note that now we don't have to assume the max is nondegenerate! If it is attained at a point (x_0, T) of the top edge t = T, we still have $v_{xx}(x_0, T) \le 0$,

and $v(x_0, t) \le v(x_0, T)$ for $t < t_0$, so $v_t(x_0, T) \ge 0$. But then $v_t - kv_{xx} \ge 0$ at (x_0, T) , again a contradiction.

Thus $\max_R v = \max_{\partial_p R} v \leq \max_{\partial_p R} u + CL^2$. Since $\max_R u = \max_R (v - Cx^2) \leq \max_R v$, we conclude $\max_R u \leq \max_{\partial_p R} u + CL^2$. Now let $C \to 0$ to conclude $\max_R u \leq \max_{\partial_p R} u$. The opposite inequality is clear, since $\partial_p R \subset R$. Hence they are equal.

A similar proof applies to the minimum.

The maximum principle leaves open the possibility that the maximum (or minimum) values of u are attained not just on the parabolic boundary, but also elsewhere on R. This in fact cannot happen (unless u is constant in R), but is harder to prove.

Strong maximum principle. If u is a solution of the heat equation in a rectangle R on the upper half-plane, the maximum and minimum values of u in R are attained only on $\partial_p R$, unless u is constant on R.

For a proof, see [Protter-Weinberger].

Application. The maximum principle immediately implies uniqueness of solutions of the non-homogeneous Dirichlet problem in [0, L]:

$$u_t - ku_{xx} = f(x,t)$$
 in $R = [0, L] \times [0, T], u(0,t) = g(t), u(L,t) = h(t), u(x,0) = u_0(x).$

Just observe the if u_1 and u_2 are two solutions of this problem in [0, L], their difference $w = u_1 - u_2$ is a solution of $w_t = kw_{xx}$ in the same interval, with zero boundary conditions and zero initial condition. Thus its maximum and minimum values on $\partial_p R$ are both zero, so $w \equiv 0$ on $\partial_p R$, and by the maximum/minimum principle it follows that $w \equiv 0$ in R, so $u_1 \equiv u_2$ in R.

Question: How would you use the Maximum Principle to show uniqueness for the non-homogeneous Neumann problem in [0, L]? (That is, $u_x(0, t) = g(t), u_x(L, t) = h(t)$). Note that u_x is also the solution of a non-homogeneous heat equation, if u is.

PROBLEMS.

1. Solve the heat equation $u_t - u_{xx} = 0$ on the real line, with initial exponential initial data $u_0(x) = e^{ax}$, where $a \in \mathbb{R}$ is a constant. (Answer: $e^{t\bar{a^2}+ax}$

Hint: In the integral with the heat kernel, complete squares to obtain:

$$\frac{(x-y)^2}{4t} - ay = (\frac{x-y}{\sqrt{4t}} + \sqrt{t}a)^2 - ta^2 - ax,$$

- then make the change of variables $z = \frac{x-y}{\sqrt{4t}} + \sqrt{t}a$. 2. Solve the heat equation $u_t u_{xx} = 0$, for the following two initial conditions:
 - (i) $u_0(x) = 1$ for x > 0 and $u_0(x) = -2$ for x < 0.
- (ii) $u_0(x) = x, x < 0 \text{ or } x > 4; u_0(x) = x + 2, 0 < x < 4.$ (*Hint:* write $u_0(x) = x + 2(\theta_a(x) - \theta_b(x))$ for suitable a and b, then use linearity.)
- 3. [Strauss] Consider the solution $1 x^2 2t$ of $u_t u_{xx} = 0$. Find the locations of its maximum and minimum points in the closed rectangle $\{0 \le x \le 1, 0 \le t \le T\}.$
- **4.**[Strauss] Consider the diffusion equation $u_t = u_{xx}$ on the interval [0, 1], with initial condition $u_0(x) = 4x(1-x)$ and boundary conditions u(0,t) =u(1,t) = 0.
 - (i) Show that 0 < u(x,t) < 1 for all t > 0 and 0 < x < 1.
- (ii) Show that u(x,t) = u(1-x,t) for all $t \ge 0$ and $x \in [0,1]$. (Hint: uniqueness.
- (iii) Use the energy method to show that $\int_0^1 u^2 dx$ is a strictly decreasing function of t.
- **5.** [Strauss] Solve the diffusion equation $u_t = u_{xx}$ on the real line, with initial condition:

$$u_0(x) = e^{ax}, x > 0; u_0(x) = 0, x < 0.$$

Hint: Use the same trick as in problem 1. $Answer:e^{ta^2+ax}ERF(\frac{x}{\sqrt{4t}}-\sqrt{t}a)$.

6.[Strauss] Solve the diffusion equation $u_t - u_{xx} = 0$ on the real line with initial condition:

$$u_0(x) = x^2 - 3x + 7.$$

Hint: Show that u_{xxx} solves the heat equation with initial data zero, hence (by uniqueness) is the identically zero function for each t > 0. This means:

$$u(x,t) = A(t)x^2 + B(t)x + C(t).$$

Now substitute back in the equation to find the coefficients A(t), B(t), C(t).

Remark. Clearly this method applies to any initial condition that is a polynomial function of x. In fact, you can show that if $u_0(x)$ is a polynomial of degree d, then so is u(x,t), for each t>0.

5. Stability and energy.

5.1 Norms in function spaces. A norm in a vector space V is an assignment $v\mapsto ||v||$ of a nonnegative real number to each vector in $v\in V$, satisfying: (i) ||v||=0 only when v=0; ||cv||=|c|||v||, for each $v\in V$ and each $c\in \mathbb{R}$; (iii) $||v+w||\leq ||v||+||w||$, for each $v,w\in V$ (triangle inequality.)

Examples. In finite dimensions (that is, in \mathbb{R}^n), the best-known example is the euclidean norm $||\cdot||_2$: if $v=(x_1,\ldots,x_n)\in\mathbb{R}^n$:

$$||v||_2 = (x_1^2 + \dots + x_n^2)^{1/2}.$$

For any p > 0, we can define analogously:

$$||v||_p = (|x_1|^p + \ldots + |x_n|^p)^{1/p}$$

(why do we need the absolute values?) It turns out the $||\cdot||_p$ are norms, but only for $p \ge 1$ (the problem is the triangle inequality.) The following is also a norm in \mathbb{R}^n :

$$||v||_{\infty} = \max\{|x_1|, \dots, |x_n|\}.$$

Exercise. For any norm, we have the 'unit ball': $B = \{v \in V; ||v|| \leq 1\}$. Sketch the unit balls for the norms in \mathbb{R}^2 : $||\cdot||_1, ||\cdot||_2, ||\cdot||_3$ and $||\cdot||_{\infty}$.

Exercise. Show that in \mathbb{R}^n : $\lim_{p\to\infty} ||v||_p = ||v||_{\infty}$. (This explains the notation.)

Remark. It is a fact of Analysis that, in a finite-dimensional vector space V, any two norms $||\cdot||$ and $||\cdot||'$ are equivalent, in the sense that there exists a constant C > 1 so that:

$$\forall v \in V : \frac{1}{C} ||v||' \le ||v|| \le C||v||'.$$

(In particular, convergence of a sequence to a given limit is independent of the choice of norm.) This is definitely *false* in infinite dimensions. (A simple example is given below.)

Here we are primarily concerned with infinite-simensional vector spaces of functions, for the moment subspaces of the space of piecewise continuous, bounded functions on the real line or on an interval. On $C_b(\mathbb{R})$ or $C_b([a,b])$ (continuous and bounded, or even piecewise continuous and bounded) we have the 'uniform norm':

$$||f||_{\infty} = \sup_{x \in I} |f(x)|,$$

where $I = \mathbb{R}$ or I = [a, b], and sup ('supremum') is the smallest M > 0 so that $|f(x)| \leq M$ for all $x \in I$ (often, but not always, this is the maximum of |f(x)| in I).

We also have the ' L^p norms' on the space of piecewise continuous functions on a bounded interval [a, b]:

$$||f||_p = (\int_a^b |f|^p (x) dx)^{1/p}, p \ge 1.$$

Of these by far the most important is the L^2 norm, which is associated to the L^2 inner product:

$$||f||_2 = \langle f, f \rangle^{1/2}$$
, where $\langle f, g \rangle = \int_a^b f(x)g(x)dx$.

Remark. (i) Something is being 'swept under the rug' here. If a piecewise continuous function has zero L^p norm, it is not quite true that it is the zero function (it could be nonzero at finitely many points in [a, b]. If we consider only continuous functions (one-sided continuous at a and b), this problem disappears (but this solution is less satisfying than it looks.)

(ii) Note that for any continuous function f in [a, b] we have:

$$||f||_2 = (\int_a^b f^2(x)dx)^{1/2} \le (b-a)^{1/2}||f||_{\infty}.$$

However, we don't have an inequality in the other direction. For the sequence $f_n(x) = x^n$ in [0,1], we have $||f_n||_2 = (2n+1)^{-1/2} \to 0$ but $||f_n||_{\infty} = 1$ for all n. This shows these two norms in C[0,1] are not equivalent.

5.2 First energy argument. We show the L^2 norm of solutions of the heat equation is decreasing in time. Let u(x,t) be a solution of $u_t - ku_{xx} = 0$ in the usual spaces $V_D[0,L], V_N[0,L], V_{per}[-L,L]$. Integrating by parts we find:

$$\frac{d}{dt} \int_0^L u^2 dx = 2 \int_0^L u u_t dx = 2k \int_0^L u u_{xx} dx = -\int_0^L u_x^2 dx + u u_x \Big|_0^L,$$

and the last term is zero in any of the usual spaces. This shows $\int_0^L u^2 dx$ is decreasing in time, unless u is a constant solution. This implies the following stability estimate for solutions u^1, u^2 of the heat equation in V_D, V_N or V_{per} with initial conditions u_0^1, u_0^2 (resp.):

$$||u^1(\cdot,t) - u^2(\cdot,t)||_2 \le ||u_0^1 - u_0^2||_2.$$

(Recall a *stability estimate* for a PDE shows that if the data of the problem are 'close' (in a given norm), then the solutions are also 'close', for any given t > 0.)

Exercise. Can you use this method to show the L^p norms of the solution (for $p \geq 2$) are also decreasing in time?

5.3 Second energy argument. One way to define an "energy" for a function on an interval is to measure the deviation from being a constant. A simple way to do this is to set:

$$E[f] = \frac{1}{2} \int_{a}^{b} (f_x)^2 dx, \quad f \in C^1_{pw}[a, b].$$

 (C_{pw}^1) : continuous, with piecewise continuous derivative). Thus E[f] = 0 exactly if f is constant. Let's compute the time derivative of the energy for a solution of the heat equation $u_t - ku_{xx} = 0$ in an interval [a, b], in one of the usual spaces V_D, V_N, V_{per} :

$$\frac{dE[u]}{dt} = \int_{a}^{b} u_{x} u_{xt} dx = -\int_{a}^{b} u_{xx} u_{t} dx + u_{x} u_{t}|_{x=a}^{x=b}$$
$$= -k \int_{a}^{b} (u_{xx})^{2} dx \le 0,$$

since the boundary term $u_x u_t|_a^b$ vanishes for u in V_D, V_N or V_{per} . Thus the energy is decreasing in time (unless u is constant, in which case its energy is zero).

One might be tempted to use the energy to define a norm, but that doesn't work, since the constant functions have zero energy. It would work as a norm in V_D , since zero is the only constant in V_D . One option is to add the L^2 integral to the energy; this defines the ' H^1 norm':

$$||f||_{H^1} = (\int_a^b f^2 dx + \int_a^b f_x^2 dx)^{1/2}.$$

This norm is associated to the H^1 inner product in $C^1_{pw}[a,b]$:

$$\langle f, g \rangle_{H^1} = \int_a^b fg dx + \int_a^b f_x g_x dx.$$

It then follows from the above that the H^1 norm is decreasing in time for solutions of the heat equation, in particular:

$$||u(\cdot,t)||_{H^1} \le ||u_0||_{H^1}.$$

This is a different 'stability estimate' for the heat equation.

Important Remark. There is a deeper connection between the energy E[f] and the heat equation. Consider a one-parameter family of functions in a vector space V[a, b] in the interval [a, b], with 'initial velocity' $g \in V[a, b]$:

$$f(\cdot, s) \in V[a, b], s \in I \subset \mathbb{R}, \frac{d}{ds} f_{s|s=0} = g \in V[a, b].$$

Then:

$$\frac{d}{ds}E[f_s]_{|s=0} = \int_a^b f_{0x}g_x dx = -\int_a^b f_{0xx}g dx + f_{0x}g|_a^b.$$

If we take V of Dirichlet, Neumann or periodic type, the boundary term vanishes. Endowing V with the L^2 inner product, we may write this as:

$$\frac{d}{ds}E[f_s]_{|s=0} = -\langle f_{0xx}, g \rangle_{L^2} = \langle L[f_0], g \rangle.$$

By analogy with finite-dimensional vector calculus, we may say that the left-hand side is the directional derivative of E at f_0 in the direction given by g. Since g is arbitrary in V, we could say the "gradient vector" of E at f_0 is $-f_{0xx} = L[f_0]$. Thus the heat equation $u_t = u_{xx}$ corresponds to the gradient flow:

$$u_t = -\operatorname{grad} E(u) = -L[u]$$

Recalling the usual interpretation of gradient flows, this suggests the heat equation decreases the energy of a function at the fastest possible rate. (All of this can be made rigorous.)

6. The heat equation with boundary conditions.

We consider first the case of Dirichlet, Neumann or periodic boundary conditions on a bounded interval, corresponding to the function spaces $V_D[0, L], V_N[0, L], V_{per}[-L, L]$. Denote by V any of these spaces, endowed with the L^2 inner product. Given $u_0 \in V$, we consider the problem:

$$u_t - ku_{xx} = 0, u(\cdot, t) \in V, u(x, 0) = u_0(x).$$

We suppose V admits an *orthonormal* basis φ_n of eigenfunctions of the differential operator $L[f] = -f_{xx}$. As for the wave equation, eigenfunctions evolve by multiplication by a function of t:

$$L[\varphi] = \lambda \varphi, u(x,0) = \varphi(x) \Rightarrow u(x,t) = A(t)\varphi(x), A(0) = 1.$$

and the heat equation implies A(t) solves an ODE:

$$A'(t)\varphi(x) = u_t = u_{xx} = -L[u] = -A(t)L[\varphi] = -\lambda A(t)\varphi \Rightarrow A'(t) = -\lambda A(t).$$

Thus
$$A(t) = e^{-\lambda t}$$
 and $u(x,t) = e^{-\lambda t}\varphi(x)$.

A general initial condition $u_0 \in V$ admits a (formal) expansion in terms of eigenfunctions:

$$u_0(x) \sim \sum_{n=1}^{\infty} A_n \varphi_n(x), \quad L[\varphi_n] = \lambda_n \varphi_n,$$

where:

$$A_n = \langle u_0, \phi_n \rangle.$$

The corresponding solution of the heat equation then has the (formal) expansion:

$$u(x,t) \sim \sum_{n=1}^{\infty} A_n e^{-\lambda_n t} \varphi_n(x).$$

Using the definition of the L^2 inner product, we find (if the interval is [0, L], say):

$$u(x,t) \sim \sum_{n=1}^{\infty} \int_{0}^{L} e^{-\lambda_n t} u_0(y) \varphi_n(y) \varphi_n(x) dy,$$

and assuming integration and infinite sum may be interchanged, we write this in familiar form:

$$u(x,t) \sim \int_0^L \sum_{n=1}^\infty e^{-\lambda_n t} \varphi_n(x) \varphi_n(y) u_0(y) dy = \int_0^L h_V(x,y,t) u_0(y) dy,$$

where we have set:

$$h_V(x, y, t) = \sum_{n=1}^{\infty} e^{-\lambda_n t} \varphi_n(x) \varphi_n(y),$$

the 'formal heat kernel' in the function space V.

We'll develop this explicitly for $V_D[0,L]$ and $V_{per}[-L,L]$, leaving the case of V_N for the exercises. In $V_D[0,L]$, the eigenfunction expansion corresponds to the Fourier sine series:

$$u_0(x) \sim \sum_{n=1}^{\infty} b_n \sin(\frac{n\pi x}{L}), \quad b_n = \frac{2}{L} \int_0^L u_0(y) \sin(\frac{n\pi y}{L}) dy.$$

Since the eigenvalues are $\lambda_n = (n\pi/L)^2$, the solution is:

$$u(x,t) \sum_{n=1}^{\infty} b_n e^{-\frac{n^2 \pi^2}{L^2} t} \sin(\frac{n\pi x}{L})$$

$$\sim \int_0^L \frac{2}{L} \sum_{n=1}^{\infty} e^{-\frac{n^2 \pi^2}{L^2} t} \sin(\frac{n\pi x}{L}) \sin(\frac{n\pi y}{L}) u_0(y) dy$$

$$= \int_0^L h_D(x, y, t) u_0(y) dy,$$

where $h_D(x, y, t)$, the 'formal heat kernel in [0, L]', is given by:

$$h_D(x, y, t) = \frac{2}{L} \sum_{n=1}^{\infty} e^{-\frac{n^2 \pi^2}{L^2} t} \sin(\frac{n\pi x}{L}) \sin(\frac{n\pi y}{L}).$$

In fact, using $\sin a \sin b = \frac{1}{2} [\cos(a-b) - \cos(a+b)]$ we have:

$$h_D(x,y,t) = k_D(x-y,t) - k_D(x+y,t), \quad k_D(x,t) = \frac{1}{L} \sum_{n=1}^{\infty} e^{-\frac{n^2 \pi^2}{L^2} t} \cos(\frac{n\pi x}{L}).$$

(Compare with the Dirichlet kernel for the half-line, described below.) Observe the following:

- (i) $h_D(x, y, t) = h_D(y, x, t)$;
- (ii) $h_D(x,\cdot,t) \in V_D[0,L]$ for all (x,t) in the upper half-plane $\{t>0\}$. (Also $h_D(\cdot,y,t) \in V_D[0,L]$, for each (y,t).)

Turning to periodic boundary conditions, we consider the evolution of $u_0 \in V_{per}[-L, L]$ under $u_t - u_{xx} = 0$. The eigenfunction expansion corresponds to the full Fourier series of u_0 :

$$u_0(x) \sim \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos(\frac{n\pi x}{L}) + b_n \sin(\frac{n\pi x}{L}),$$

where:

$$a_n = \frac{1}{L} \int_{-L}^{L} \cos(\frac{n\pi y}{L}) u_0(y) dy, n \ge 0; \quad b_n = \frac{1}{L} \int_{-L}^{L} \sin(\frac{n\pi y}{L}) u_0(y) dy, n \ge 1.$$

(Note the constant term $a_0/2$ is the average value of u_0 over [-L, L].)

The formal Fourier series of the solution is then:

$$u(x,t) \sim \frac{a_0}{2} + \sum_{n=1}^{\infty} e^{-\frac{n^2\pi^2}{L^2}t} [a_n \cos(\frac{n\pi x}{L}) + b_n \sin(\frac{n\pi x}{L})].$$

Substituting the expressions for the Fourier coefficients and formaly exchanging integration and infinite sum, we find:

$$u(x,t) \sim \frac{1}{L} \int_{-L}^{L} \{ \frac{1}{2} + \sum_{n=1}^{\infty} e^{-\frac{n^2 \pi^2}{L^2} t} \left[\cos(\frac{n\pi x}{L}) \cos(\frac{n\pi y}{L}) + \sin(\frac{n\pi x}{L}) \sin(\frac{n\pi y}{L}) \right] \} u_0(y) dy,$$

or:

$$u(x,t) \sim \int_{-L}^{L} h_{per}(x-y,t)u_0(y)dy,$$

where $h_{per}(x,t)$, the 'formal heat kernel in $V_{per}[-L,L]$ ', is given by:

$$h_{per}(x,t) = \frac{1}{2L} + \frac{1}{L} \sum_{n=1}^{\infty} e^{-\frac{n^2 \pi^2}{L^2} t} \cos(\frac{n\pi x}{L}).$$

Note $h_{per}(x,t)$ is even in x, and in $V_{per}[-L,L]$ for each t>0. We also observe the relation with the Dirichlet heat kernel in [0,L]:

$$h_D(x, y, t) = h_{per}(x - y, t) - h_{per}(x + y, t), \quad h_{per}(x, t) = \frac{1}{2L} + k_D(x, t).$$

Exercise. Write down the corresponding development in $V_N[0, L]$, including the heat kernel in $V_N[0, L]$, and its relation with h_{per} . Hint: recall the eigenfunction expansion in $V_N[0, L]$ corresponds to the Fourier cosine series:

$$u_0(x) \sim \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos(\frac{n\pi x}{L}), \quad a_n = \frac{2}{L} \int_0^L u_0(y) \cos(\frac{n\pi y}{L}) dy, n \ge 0.$$

Problems on the half-line. As for the wave equation, boundary value problems on the half-line $\{x > 0\}$ can be solved by extending the initial data to the whole real line. Consider the Dirichlet problem:

$$u_t - ku_{xx} = 0$$
 on $\{x > 0, t > 0\}, u(x, 0) = u_0(x), u(0, t) = 0$ for all $t > 0$.

If we want continuous solutions up to t = 0, the compatibility condition $u_0(0) = 0$ is required (we assume u_0 is defined, continuous and bounded on $\{x \ge 0\}$).

Denote by u_0^o the odd extension of u_0 to the real line (that is, $u_0^o(x) = -u_0(-x)$ if x < 0). This extension is continuous, since $u_0(0) = 0$. We can write down the solution using the heat kernel:

$$u(x,t) = \int_{-\infty}^{\infty} h(x-y,t)u_0^o(y)dy,$$

but it is useful to have an expression using only the original u_0 . The integral on the negative half-line can be rewritten using the change of variable $y \to z = -y$, to give:

$$u(x,t) = \int_0^\infty [h(x-y,t) - h(x+y,t)]u_0(y)dy.$$

PROBLEMS.

- 1. Solve $u_t = u_{xx}$ on the half-line $\{x > 0\}$, with Dirichlet boundary condition u(0,t) = 0 and initial condition $u_0(x) = \sinh x = \frac{1}{2}(e^x e^{-x})$.
- **2.** (i) Find a formula for the solution of the Neumann problem on the half-line $\{x > 0\}$, with boundary condition $u_x(0,t) = 0$ and initial condition $u_0(x)$, where $u'_0(x) = 0$. Write down the answer in the form:

$$u(x,t) = \int_0^\infty h_n(x,y,t)u_0(y)dy$$

(that is, find the 'Neumann heat kernel' $h_N(x, y, t)$ for the half-line.

- (ii) Solve $u_t = u_{xx}$ on $\{x > 0\}$, with Neumann boundary conditions and initial condition $u_0(x) = \cosh(x) = \frac{1}{2}(e^x + e^{-x})$.
- **3.** Let u be a solution of the heat equation in $V_N[0, L]$. Use the energy method to show the integral $\int_0^L (u \bar{u})^2 dx$ is decreasing in t (unless $u \equiv u_0$ is constant). Here \bar{u} is the average value of the solution over the interval [0, L] (which is independent of t).
- **4.** The function $u_0(x) = \sin^2 x$ is in all three spaces $V_D[0, \pi], V_N[0, \pi], V_{per}[-\pi, \pi]$. Solve the heat equation $u_t = u_{xx}$ with initial condition u_0 , in each of these spaces. *Hint:* In V_N and V_{per} , u_0 is a finite linear combination of eigenfunctions; to solve the problem in V_D , compute its Fourier sine series.
- 5. Suppose u(x,t) solves the heat equation with Neumann boundary conditions in $[0,\pi]$, and the initial condition u_0 is a finite linear combination of eigenfunctions:

$$u_0(x) = \sum_{n=0}^{N} a_n \cos nx.$$

Find constants C > 0 and $\lambda > 0$ so that $|u(x,t) - \bar{u}| \le Ce^{-\lambda t}$.

6. Find an expression (as an infinite series of functions) for the heat kernel in $V_N[0,\pi]$, and its relation with the periodic heat kernel in $[-\pi,\pi]$, h_{per} . Hint: recall the eigenfunction expansion in $V_N[0,L]$ corresponds to the Fourier cosine series:

$$u_0(x) \sim \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos nx$$
 $a_n = \frac{2}{\pi} \int_0^{\pi} u_0(y) \cos(ny) dy, n \ge 0.$