HEAT AND GEOMETRY

JULIE ROWLETT

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In this lecture we're going to construct the heat kernel on a closed RIemannian manifold. It will probably feel like we've run a marathon after having done so. Let's begin by defining the heat kernel on a closed manifold and proving that if it exists, it is unique.

Definition 1. A heat kernel, $H(t, x, y)$ is a function in $\mathcal{C}^2((0, \infty) \times M \times M)$ which satisfies

$$\Xi H(t, x, y) = 0 \quad \forall t > 0,$$
$$\lim_{t \to 0} H(t, x, y) f(y) dy = f(x)$$

for all continuous functions f on M.

p:uniqueness **Proposition 2.** *If a heat kernel exists, then it is symmetric in its space variables, and it is unique.*

Proof: First, we show that if a heat kernel exists, then it is symmetric in the space variables, hence there is no weird question about which variable Δ in Ξ is acting upon. It is either acting on x or y, and it don't matter which. Let us assume that H is a heat kernel. We apply Stokes's theorem (integration by parts) using the fact that M is a closed manifold to kill the boundary terms, obtaining

$$0 = \int_M \Delta_y H(\tau, x, y) \cdot H(t - \tau, z, y) dy - H(\tau, x, y) \Delta_y H(t - \tau, z, y) dy.$$

Next we apply the heat equation to turn the Laplacians into time derivatives:

$$0 = \int_M -\partial_\tau H(\tau, x, y) H(t - \tau, z, y) dy - H(\tau, x, y) \partial_\tau H(t - \tau, z, y) dy.$$

By Leibniz's rule (basically the product rule) this is equivalent to

$$0 = -\partial_\tau \int_M H(\tau, x, y) H(t - \tau, z, y) dy.$$

If you're bothered by this exchange of limits, remember that we're on a compact manifold, and H is $\mathcal{C}^2$ in both space and time variables, so it's legit. Absolute convergence everywhere. Now, we integrate this vanishing expression and still obtain zero:

$$0 = \int_0^t d\tau \left(\partial_\tau \int_M H(\tau, x, y) H(t - \tau, z, y) dy \right).$$

This is essentially doing a Lebesgue integral in τ because although something funky could happen right at $\tau = 0$ and $\tau = t$, but that's only one point (measure zero set), and so the integral of something which vanishes except for possibly at a set of measure zero is still zero. So, now we compute this by noting that by the definition of the heat kernel and its regularity

$$\lim_{s\to 0}\int_M H(t,x,y)H(s,z,y)dy = H(t,x,z), \quad \lim_{s\to 0}\int_M H(s,x,y)H(t,z,y)dy = H(t,z,x).$$

It may look confusing, but what's going on is the heat kernel $H(s,z,y)$ is acting on $H(t,x,y)$ which is viewed as a function of y for fixed x and t. So, by definition of the heat kernel, we obtain $H(t,x,z)$ in the first limit. A similar idea elucidates the second limit. We therefore obtain by the above argument together with the fundamental theorem of calculus that

$$\begin{aligned} 0 &= \int_0^t d\tau \left(\partial_\tau \int_M H(\tau,x,y)H(t-\tau,z,y)dy\right) \\ &= \lim_{t-\tau\to 0}\int_M H(\tau,x,y)H(t-\tau,z,y)dy - \lim_{\tau\to 0}\int_M H(\tau,x,y)H(t-\tau,z,y)dy \\ &= H(t,x,z) - H(t,z,x). \end{aligned}$$

Since the choice of z and x is arbitrary, we get that

$$H(t,x,z) = H(t,z,x) \quad \forall x\in M, \quad z\in M.$$

Therefore, heat kernels are symmetric in the space variables.

Now, let us assume that H and K are both heat kernels. Using a similar argument as above,

uniqueness

$$\begin{aligned} &\int_0^t ds\partial_s \int_M H(s,x,y)K(t-s,y,z)dy \\ &= \lim_{\tau\to 0}\left[\int_M H(t-\tau,x,y)K(\tau,y,z)dy - \int_M H(\tau,x,y)K(t-\tau,y,z)dy\right] \\ &= H(t,x,z) - K(t,x,z). \end{aligned} \tag{1.1}$$

So, the idea is to play around with the expression involving the ∂_s above, use the heat equation and probably symmetry in the variables, to show that the expression vanishes. Then we'll get that $H(t,x,z) - K(t,x,z)$ is identically zero, so they're the same. So, let's distribute the ∂_s inside the integral (don't worry, everything converges just fine, if you're stressed about it, then prove it yourself as an **exercise!**).

$$\int_0^t ds\left[\int_M \partial_s H(s,x,y)\cdot K(t-s,y,z)dy + \int_M H(s,x,y)\partial_s K(t-s,y,z)dy\right].$$

We substitute the time derivatives for Laplacians using the heat equation! So, our expression becomes

$$\int_0^t ds\left[\int_M -\Delta_x H(s,x,y)\cdot K(t-s,y,z)dy + \int_M H(s,x,y)\Delta_y K(t-s,y,z)dy\right].$$

By symmetry in the variables,

$$-\Delta_x H(s,x,y) = -\Delta_y H(s,x,y)|_{(s,y,x)}.$$

This might seem a little weird, so I try to explain. The idea is if you differentiate in the first space variable, then plop in (x,y) it's the same as if you differentiate in the second space variable, then plop in (y,x):

$$-\Delta_{x_1}H(s,x_1,x_2)|_{(x,y)} = -\Delta_{x_2}H(s,x_1,x_2)|_{(y,x)}.$$

So, we use this switcharoo to change

$$\int_M -\Delta_x H(s,x,y)\cdot K(t-s,y,z)dy = \int_M -\Delta_y H(s,x,y)|_{(y,x)} \cdot K(t-s,y,z)dy.$$

Now we integrate by parts twice to jam the Lapalcian onto K, obtaining

$$-\int_M H(s,y,x)\Delta_y K(t-s,y,z)dy = -\int_M H(s,x,y)\Delta_y K(t-s,y,z)dy.$$

Above we used the symmetry in the space variables on H. So, now our expression becomes:

$$\int_0^t ds\left[-\int_M H(s,x,y)\Delta_y K(t-s,y,z)dy + \int_M H(s,x,y)\Delta_y K(t-s,y,z)dy\right] = 0.$$

Voilà! It vanishes, independently of the choice of x and z. Hence, (1.1) vanishes for all x and z, showing that H and K are indeed the same.

1.1. **The heat kernel on a closed Riemannian manifold.** The manifold is compact, so there exists a uniform constant $\varepsilon > 0$ such that for any $x \in M$ the exponential map at x is a diffeomorphism from the ball of radius ε in the tangent space onto $B_x(\varepsilon)$. Fix a point $x \in M$. For any $y \in B_x(\varepsilon)$ the Riemannian distance, $d(x,y)$, from x to y satisfies $d(x,y) < \varepsilon$. Let

$$U_\varepsilon = \{(x,y) \in M \times M \mid y \in B_x(\varepsilon)\ \}.$$

Let

$$G(t,x,y) = (4\pi t)^{-n/2} e^{-\frac{d^2(x,y)}{4t}}$$

be the direct analogue of the Euclidean heat kernel on M which belongs to $C^\infty(\mathbb{R}^+ \times U_\varepsilon)$. Set

$$u(t,x,y) = u_0(x,y) + \ldots + u_k(x,y)\, t^k$$

where the functions $u_i(x,y)$ are to be determined. Define

$$S = S_k(t,x,y) = G(t,x,y)\ u(t,x,y).$$

So, for $(x,y) \in U_\varepsilon$ we compute

$$= \frac{\partial}{\partial t} S = G \cdot \left(\left(-\frac{n}{2t} + \frac{r^2}{4t^2} \right)(u_0 + \ldots + t^k u_k) + (u_1 + 2tu_2 + \ldots + kt^{k-1}u_k) \right).$$

where $r = d(x,y)$. Denote the inner product on M by $\langle \cdot, \cdot \rangle$. The Leibniz (product) rule works on a Riemannian manifold in the same way as it works in $\mathbb{R}^n$, that is

$$\Delta(h \cdot g) = (\Delta h)g + h\Delta g - 2\langle \nabla h, \nabla g \rangle.$$

We then compute

$$\Delta_y S = (\Delta G)(u_0 + \ldots + u_k t^k) - 2\langle dG, d(u_0 + \ldots + u_k t^k)\rangle + G\Delta(u_0 + \ldots + u_k t^k).$$

Exercise 1. *Let r be the radial coordinate in exponential polar coordinates centered at p. If f is a function of r alone, then show that*

$$\Delta f = -\frac{\partial^2}{\partial r^2} f - \left(\frac{n-1}{r} + \frac{D'}{D} \right) \partial_r f,$$

where

$$D = det(d\exp_x)$$

is the determinant of the Riemannian volume form centered at x, and $D' = \partial D/\partial r$ is its derivative with respect to the radial function $r(y) = d(x,y)$. (Hint: This is rose [3, Theorem 2.63]*.)*

Since our G is a function which depends only on $r = d(x,y)$ (in the eyes of the Laplacian on M which does not care about the time dependence), we therefore have

$$\Delta G = -\frac{\partial^2 G}{\partial r^2} - \frac{\partial G}{\partial r}\left(\frac{D'}{D} + \frac{n-1}{r}\right).$$

We compute that

$$\partial_r G = -\frac{r}{2t}G, \quad \partial_r^2 G = -\frac{G}{2t} + \frac{r^2}{4t^2}G,$$

so

$$\Delta G = \frac{G}{2t} - \frac{r^2}{4t^2}G + \frac{r}{2t}G\left(\frac{D'}{D} + \frac{n-1}{r}\right) = \left(\frac{n}{2t} - \frac{r^2}{4t^2}\right)G + \frac{r}{2t}\frac{D'}{D}G.$$

We then also compute

$$\langle dG, D(u_0 + \ldots + u_k t^k)\rangle = \langle \partial_r G dr + \partial_\theta G d\theta, d(u_0 + \ldots + u_k t^k)\rangle$$
$$= \langle \partial_r G dr, \partial_r u_0 dr + \partial_\theta u_0 d\theta + \ldots + t^k \partial_r u_k dr + \partial_\theta u_k d\theta\rangle.$$

By the choice of local frame, the vector fields dr and $d\theta$ are orthogonal, so the terms with $\langle ...dr, ...d\theta\rangle$ vanish whereas $\langle dr, dr\rangle = 1$, and we just get

$$\partial_r G\left(\partial_r u_0 + \ldots + t^k \partial_r u_k\right) = -\frac{r}{2t}G\left(\partial_r u_0 + \ldots + t^k\partial_r u_k\right).$$

Hence

$$\Delta_y S_k = G\left[\left(\frac{n}{2t} - \frac{r^2}{4t^2}\right) + \frac{r}{2t}\frac{D'}{D}\right](u_0 + \ldots + u_k t^k) + \frac{r}{t}G\left(\partial_r u_0 + \ldots + t^k \partial_r u_k\right) + G\Delta(u_0 + \ldots + u_k t^k).$$

Recalling

$$\frac{\partial}{\partial t}S = G\cdot\left(\left(-\frac{n}{2t} + \frac{r^2}{4t^2}\right)(u_0 + \ldots + t^k u_k) + (u_1 + 2tu_2 + \ldots + kt^{k-1}u_k)\right),$$

we get awesome cancellation:

heat1
$$\left(\frac{\partial}{\partial t} + \Delta_y\right)S_k = G\Big[u_1 + \ldots + kt^{k-1}u_k + \frac{r}{2t}\frac{D'}{D}(u_0 + \ldots + t^k u_k)$$
$$+ \frac{r}{t}\left(\frac{\partial u_0}{\partial r} + \ldots + t^k\frac{\partial u_k}{\partial r}\right) + \Delta_y u_0 + \ldots + t^k \Delta_y u_k\Big] \quad (1.2)$$

To obtain the parametrix we will choose u_i inductively such that the coefficient of t^i vanishes for $-1 \le i \le k-1$. The coefficient of t^{-1} will vanish if we set

$$\frac{r}{2}\frac{D'}{D}u_0 + r\frac{\partial u_0}{\partial r} = 0.$$

This first order differential equation has a smooth solution for $r < \varepsilon$ given by

$$u_0(x,y) = D^{-1/2}(y)$$

which is a smooth function on U_ε independently of f and satisfies

$$u_0(x,x) = 1.$$

For t^{i-1} we obtain the equation

$$i\,u_i + \frac{r}{2}\frac{D'}{D}u_i + r\frac{\partial u_i}{\partial r} + \Delta_y u_{i-1} = 0.$$

Letting $x(s)$ be the unit speed geodesic from x to y for $s \in [0, r]$ with $x(0) = x$ and $x(r) = y$, we may obtain a solution to the above equation from the integral equation

u_i
$$u_i(x, y) = -r^{-i}(x, y) D^{-1/2}(y) \int_0^r D^{1/2}(x(s)) \cdot (\Delta_{x(s)} u_{i-1})(x, x(s)) \cdot s^{i-1} ds. \tag{1.3}$$

In the above x stays fixed, and y varies along the geodesic from x. Observe that the functions u_i are smooth on $M \times M$.

As a result,

heat2
$$\left(\frac{\partial}{\partial t} + \Delta_{f,y}\right) S_k = G(t, x, y)\, t^k\, \Delta_y u_k(x, y) \tag{1.4}$$

Define

$$\eta(x, y) = \begin{cases} 1 & \text{on } U_{\varepsilon/2} \\ 0 & \text{on } M \times M \setminus U_\varepsilon \end{cases}$$

to be a smooth function with bounded first and second order derivatives. Then we extend S_k to $M \times M$ setting

Hk
$$h_k(t, x, y) = \eta(x, y) \cdot S_k(t, x, y) = \eta(x, y)\, G(t, x, y) \sum_{i=1}^{k} u_i(x, y)\, t^i. \tag{1.5}$$

Definition 3. A *parametrix* for the heat operator $\Xi = \partial_t + \Delta_y$ is a function $H \in \mathcal{C}^\infty(\mathbb{R}^+ \times M \times M)$ such that

(1) $\Xi H \in \mathcal{C}^0([0, \infty) \times M \times M)$ and
(2) $\lim_{t \to 0} \int_M H(t, x, y) f(y) dy = f(x)$ for all $f \in \mathcal{C}^0(M)$.

Lemma 4. *For $k > \frac{n}{2}$, h_k is a parametrix for the heat operator. Moreover, for $k > l + \frac{n}{2}$, we also have*

hkl
$$\Xi h_k \in \mathcal{C}^l([0, \infty) \times M \times M). \tag{1.6}$$

Proof: For the first statement, h_k vanishes on $M \times M \setminus U_\varepsilon$ and so Ξh_k is perfectly smooth for all t down to $t = 0$ over there. When the space variables are in $U_{\varepsilon/2}$, then we compute since η is constant over there,

$$\Xi h_k = \Xi S_k = (4\pi t)^{-n/2} t^k e^{-r^2/(4t)} \Delta u_k \to 0 \text{ as } t \to 0 \forall k > \frac{n}{2}.$$

Moreover, this is in $\mathcal{C}^l$ as long as $k > l + \frac{n}{2}$. Finally, on $U_\varepsilon \setminus U_{\varepsilon/2}$, the derivatives will hit η, so we get

$$\Xi h_k = \eta \Xi S_k - 2\langle d\eta, dS_k \rangle + (\Delta\eta) S_k = (4\pi t)^{-\frac{n}{2}} e^{-\frac{r^2}{4t}} \phi(t, x, y),$$

for some smooth function ϕ which blows up at worst like t^{-1} when $t \downarrow 0$. However, since $r > \frac{\varepsilon}{2}$ on this set, the rapid decay of the exponential (Gaussian) factor keeps everything in check as $t \to 0$, so we obtain smoothness there. All in all, what limits the smoothness is when the space variables are in $U_{\varepsilon/2}$, which is why we get the smoothness stated in (hkl 1.6).

Hence, by definition of parametrix, for any $k > \frac{n}{2}$, h_k satisfies the first condition to be a parametrix. Next, let $f \in \mathcal{C}^0(M)$. We need to show that

$$\lim_{t \downarrow 0} \int_M (4\pi t)^{-\frac{n}{2}} e^{-r^2/(4t)} \eta(x, y)(u_0(x, y) + \ldots + t^k u_k(x, y)) f(y) dy = f(x).$$

The idea is again to split the integral into the sets $d(x, y) < \varepsilon/2$ and $d(x, y) > \varepsilon/2$. For the latter, the Gaussian makes everything decay rapidly as $t \downarrow 0$ since $r =$

$d(x,y) > \varepsilon/2$ over there. On the first set, since y is so close to x, we can use the exponential map as a local coordinate chart and turn our integral into an integral over $T_xM \cong \mathbb{R}^n$, (basically we are integrating outwards from the point $x \in M$ along all directions, which corresponds to integrating over all $v \in T_xM$):

$$\int_{T_xM} (4\pi t)^{-\frac{n}{2}} e^{-r^2(0,v)/(4t)} u_i(x, \exp_x v) f(\exp_x v) D(v) dv^1 \dots dv^n,$$

where we have extended the u_i to vanish away from the ball of radius $\varepsilon/2$ about x. Here we use the fact that we've got the Euclidean heat kernel now, so that our integral converges as $t \downarrow 0$ to

$$u_i(x,x)f(x).$$

When we recall the factors of t^i attached to each u_i, and the fact that u_i is smooth and f is continuous on M which is compact (hence f is bounded), the only term which survives in

$$\lim_{t\downarrow 0} \sum_{i=0}^{k} t^i \int_{T_xM} (4\pi t)^{-\frac{n}{2}} e^{-r^2(0,v)/(4t)} u_i(x, \exp_x v) f(\exp_x v) D(v) dv^1 \dots dv^n = u_0(x,x)f(x).$$

By definition $u_0(x,x) = 1$, so we obtain the result.

To finish the construction of the heat kernel, we shall use Duhamel's formula. Let X and Y be operators acting on some Hilbert space, H of functions. Assume that there is a semigroup of bounded self-adjoint operators e^{-tX} and e^{-tY} for $t > 0$ which satisfy

$$(\partial_t + X)e^{-tX} f = 0, \quad \lim_{t\to 0} e^{-tX} f = f \quad \forall f \in H.$$

Then we have

Proposition 5 (Duhamel's formula)**.** *Provided $e^{-t(X+Y)}$ exists, we have*

$$e^{-t(X+Y)} = e^{-tX} - \int_0^t e^{-(t-s)(X+Y)} Y e^{-sX} ds.$$

Proof: Compute

$$\frac{d}{dt}\left(e^{-t(x+Y)} e^{tX}\right) = e^{-t(X+Y)}(-(X+Y))e^{tX} + e^{-t(X+Y)} e^{tX} X = -e^{-t(X+Y)} Y e^{tX}$$

due to the fact that $e^{\pm tX}$ and X commute. Therefore by the fundamental theorem of calculus,

$$e^{-t(X+Y)} e^{tX} - Id = -\int_0^t e^{-s(X+Y)} Y e^{sX} ds,$$

because at $t = 0$ the operator is the identity operator. Then applying e^{-tX} on the right to both sides we get

$$e^{-t(X+Y)} - e^{-tX} = -\int_0^t e^{-s(X+Y)} Y e^{(s-t)X} ds.$$

We make a change of variables in the integral. Let $u = t - s$. Then $s - t = -u$, $-s = u - t$, $du = -ds$, and our integral is

$$\int_t^0 e^{(u-t)(X+Y)} Y e^{-uX} du = -\int_0^t e^{-(t-u)(X+Y)} Y e^{-uX} du.$$

This is the expression in the proposition with u instead of s as the variable.

So now we define for operators on the Hilbert space, H,

$$A * B = \int_0^t A(t-s)B(s)ds.$$

With this notation,

$$e^{-t(X+Y)} = e^{-tX} - e^{-t(X+Y)} * (Ye^{-tX}).$$

Denote by $A * \ldots * A$ (m times) as A^{*m}, and define $A^{*1} + A$.

Exercise 2. *Prove by induction that*

$$e^{-t(X+Y)} = e^{-tX} + \left[\sum_{j=1}^{n} (-1)^j \left(e^{-tX} * (Ye^{-tX})^{*j} \right) \right] + (-1)^{n+1} e^{-t(X+Y)} * (Ye^{-tX})^{*n}.$$

(For a hint check [3, Corollary 3,16]*).*

For our purposes, we shall use a slightly different version of the $*$ operation, which involves both the t parameter as well as the space variables. This version is defined in the following lemma.

Lemma 6. *Let $K_k = (\partial_t + \Delta_y)h_k$. Define here*

$$A * B = \int_0^t d\theta \int_M A(\theta, x, q)B(t-\theta, q, y)dq.$$

Use this to formally define

$$Q_k = \sum_{m=1}^{\infty} (-1)^{m+1} K_k^{*m}.$$

Then, in fact Q_k exists and is in $\mathcal{C}^l(M \times M \times (0,\infty)$ if $k > l + \frac{n}{2}$. Moreover it satisfies for any fixed $T > 0$

$$|Q_k(x,y,t)| \lesssim t^{k-\frac{n}{2}} \quad \forall t \in [0,T].$$

Proof: The proof is an **exercise**. Follow the proof of [3, Lemma 3.18] for guidance.

Proposition 7. *If $P \in \mathcal{C}^0([0,\infty) \times M \times M)$ then $P * h_k \in \mathcal{C}^l([0,\infty) \times M \times M)$ for $k > l + \frac{n}{2}$. Moreover*

$$\Xi(P * h_k) = P + P * K_k, \qquad \textit{as long as } k > 2 + \frac{n}{2}.$$

Proof: It is important to note that the $*$ here is defined as in the definition of the preceding lemma. The proof of the proposition is an **exercise,** because mathematics is built on teamwork. For hints, see the proof of [3, Lemma3.21].

Theorem 8. *Let*

$$H(t,x,y) = h_k(t,x,y) - Q_k * h_k(t,x,y).$$

Then $H(t,x,y) \in C^\infty((0,\infty)\times M \times M)$*, it is independent of* k *for* $k > 2 + n/2$*, and it is the heat kernel. Moreover, the heat kernel is in* $\mathcal{C}^\infty((0,\infty)\times M\times M$*.*

Proof: Since $k > 2 + \frac{n}{2}$, it follows from the preceding lemma (yeah, teamwork!) and the definition of h_k that H is $\mathcal{C}^2$. So, we apply the heat operator to it:

$$\Xi H(t,x,y) = (\partial_t + \Delta_y)(h_k - Q_k * h_k) = K_k - Q_k - Q_k * K_k,$$

where above we have used the definition of K_k and the proposition that y'all proved (go team!). Then, writing out the definition of Q_k we're going to get some telescoping action:

$$Q_k = \sum_{m\geq 1}(-1)^{m+1}K_k^{*m} \implies -Q_k * K_k = -\sum_{m\geq 1}(-1)^{m+1}K_k^{*m+1}$$
$$= \sum_{m\geq 1}(-1)^{m+2}K_k^{*m+1} = \sum_{j\geq 2}(-1)^{j+1}K_k^{*j}.$$

So,

$$\Xi H(t,x,y) = K_k - \sum_{m\geq 1}(-1)^{m+1}K_k^{*m} + \sum_{j\geq 2}(-1)^{j+1}K_k^{*j} = K_k - (-1)^{1+1}K_k^{*1} = 0,$$

since

$$K_k^{*1} = K_k.$$

So, boo yeah, the heat equation is satisfied! Next let f be a continuous function on M.

$$\lim_{t\to 0}\int_M H(t,x,y)f(y)dy = \lim_{t\to 0}\int_M h_k(t,x,y)f(y)dy - \int_M Q_k * h_k(t,x,y)f(y)dy$$
$$= f(x) - \lim_{t\to 0}\int_M Q_k * h_k(t,x,y)f(y)dy.$$

The second term decays like $t^{k-\frac{n}{2}}$ as $t \downarrow 0$ by our collective estimates. Since $k > \frac{n}{2}$, this term vanishes in the limit, so we get that

$$\lim_{t\to 0}\int_M H(t,x,y)f(y)dy = f(x),$$

for any continuous f on M. By proposition p:uniqueness 2 and the definition of heat kernel, we see that H is unique and therefore independent of the choice of k for $k > 2 + \frac{n}{2}$. Hence, by the preceding two propositions, since h_k itself is smooth, and $Q_k * h_k \in \mathcal{C}^l((0,\infty)\times M\times M)$ for $k > l + \frac{n}{2}$, we get that H is in $\mathcal{C}^l((0,\infty)\times M \times M)$ for all l. Thus it's in $\mathcal{C}^\infty((0,\infty)\times M\times M)$. That's rather amazing, eh?

References

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