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AN ESTIMATE ON THE HESSIAN OF THE HEAT KERNEL

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ABSTRACT. Let M be a compact, connected Riemannian manifold, and let $p_t(x,y)$ denote the fundamental solution to Cauchy initial value problem for the heat equation $\frac{\partial u}{\partial t} = \frac{1}{2}\Delta u$, where Δ is the Levi–Civita Laplacian. The purpose of this note is to describe the behavior of the Hessian of $\log p_T(\,\cdot\,, y)$ for small $T > 0$.

Emphasis is given to the difference between what happens outside, where the behavior is like $\frac{1}{T}$, as opposed to at the cut locus, where it is like $\frac{1}{T^2}$.

§0: INTRODUCTION

Let M be a compact, connected, d-dimensional Riemannian manifold, denote by $\mathcal{O}(M)$ with fiber map $\pi : \mathcal{O}(M) \longrightarrow M$ the associated bundle of orthonormal frames $\mathfrak{e}$, and use the Levi–Civita connection to determine the horizontal subspace $H_{\mathfrak{e}}(\mathcal{O}(M))$ at each $\mathfrak{f} \in \mathcal{O}(M)$. Next, given $\mathbf{v} \in \mathbb{R}^d$, let $\mathfrak{E}(\mathbf{v})$ be the *basic vector field* on $\mathcal{O}(M)$ determined by properties that

$$\mathfrak{E}(\mathbf{v})_{\mathfrak{e}} \in H_{\mathfrak{e}}(\mathcal{O}(M)) \quad \text{and} \quad d\pi\mathfrak{E}(\mathbf{v})_{\mathfrak{e}} = \mathfrak{e}\mathbf{v} \quad \text{for all } \mathfrak{e} \in \mathcal{O}(M).$$

(Here, and whenever convenient, we think of $\mathfrak{e}$ as a isometry from $\mathbb{R}^d$ onto $T_{\pi(\mathfrak{e})}(M)$.) In particular, if $\{\mathbf{e}_1, \dots, \mathbf{e}_d\}$ is the standard orthonormal basis in $\mathbb{R}^d$, then we set $\mathfrak{E}_k(\mathfrak{e}) = \mathfrak{E}(\mathbf{e}_k)_{\mathfrak{e}}$. If, for $\mathcal{O} \in \mathcal{O}(d)$ (the orthogonal group on $\mathbb{R}^d$) $R_{\mathcal{O}} : \mathcal{O}(M) \longrightarrow \mathcal{O}(M)$ is defined so that

$$R_{\mathcal{O}}\mathfrak{e}\,\mathbf{v} = \mathfrak{e}\,\mathcal{O}\mathbf{v}, \quad \mathfrak{e} \in \mathcal{O}(M) \text{ and } \mathbf{v} \in \mathbb{R}^d,$$

then it easy to check that

$$dR_{\mathcal{O}}\mathfrak{E}(\mathbf{v})_{\mathfrak{e}} = \mathfrak{E}(\mathcal{O}^{\top}\mathbf{v})_{R_{\mathcal{O}}\mathfrak{e}}, \quad \mathfrak{e} \in \mathcal{O}(M) \text{ and } \mathbf{v} \in \mathbb{R}^d. \tag{0.1}$$

Given a smooth function F on $\mathcal{O}(M)$, we define $\nabla F : \mathcal{O}(M) \longrightarrow \mathbb{R}^d$, $\mathrm{Hess}\,(F) : \mathcal{O}(M) \longrightarrow \mathbb{R}^d \otimes \mathbb{R}^d$, and $\Delta F : \mathcal{O}(M) \longrightarrow \mathbb{R}$ by

$$\begin{gathered} \nabla F = \sum_1^d \mathfrak{E}_k F\, \mathbf{e}_k, \quad \mathrm{Hess}\,(F) = \big((\mathfrak{E}_k \circ \mathfrak{E}_\ell F)\big)_{1 \le k,\ell \le d} \\ \text{and} \quad \Delta F = \sum_1^d \mathfrak{E}_k^2 F. \end{gathered} \tag{0.2}$$

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In particular, when f is a smooth function on M, we set

$$\nabla f \equiv \nabla(f \circ \pi), \quad \text{Hess}\,(f) \equiv \text{Hess}\,(f \circ \pi), \quad \text{and} \quad \Delta f \equiv \Delta(f \circ \pi).$$

Starting from (0.1), it is an easy matter to check that

$$(\nabla f) \circ R_{\mathcal{O}} = \mathcal{O}^{\top} \nabla f, \quad (\text{Hess}\,(f)) \circ R_{\mathcal{O}} = \mathcal{O}^{\top} \text{Hess}\,(f)\,\mathcal{O}, \\ \text{and} \quad (\Delta f) \circ R_{\mathcal{O}} = \Delta f.$$

Hence, $|\nabla f|$, $\|\text{Hess}\,(f)\|_{\text{H.S.}}$ (the Hilbert–Schmidt norm), and Δf are all well-defined on M. In fact, Δf is precisely the action of the Levi–Civita Laplacian on f.

Now consider Cauchy initial value for the heat equation

$$\frac{\partial u}{\partial t} = \tfrac{1}{2}\Delta u, \quad t \in (0,\infty) \quad \text{with} \quad \lim_{t \searrow 0} u(t,x) = f(x), \quad x \in M.$$

By standard elliptic regularity theory, one knows that there is a unique, smooth function $(t,x,y) \in (0,\infty) \times M \times M \longmapsto p_t(x,y) \in (0,\infty)$ such that

$$u(t,x) = \int_M f(y)\, p_t(x,y)\, \lambda_M(dy), \quad (t,x) \in (0,\infty) \times M \text{ and } f \in C(M;\mathbb{R}),$$

where λ_M denotes the normalized Riemann measure on M. Moreover, because Δ is essentially self-adjoint in $L^2(\lambda_M)$, $p_t(x,y) = p_t(y,x)$.

§1: The Results

We begin by considering the logarithmic gradient $\nabla \log p_T(\,\cdot\,,y)$, for which our initial result depends only on the dimension d and the lower bound

$$\alpha \equiv \min_{\mathfrak{e} \in \mathcal{O}(M)} \min_{\mathbf{v} \in S^{d-1}} \big(\mathbf{v}, \text{Ric}(\mathfrak{e})\mathbf{v}\big)_{\mathbb{R}^d} \tag{1.1}$$

for the Ricci curvature. One (cf. [SZ]) can then show that there is a
$C(d,\alpha) < i\infty$ such that, for each $\epsilon \in (0,1)$,
(1.2)

$$\big|\nabla \log p_T(\,\cdot\,,y)\big|(x) \le \frac{\big((1+\epsilon)e^{\alpha T}\big)^{\frac{1}{2}}\rho(x,y)}{T} + \frac{C(d,\alpha)}{(\epsilon T)^{\frac{1}{2}}}, \quad (T,x,y) \in (0,1] \times M^2,$$

where we have introduced $\rho(x,y)$ to denote the Riemannian distance between x and y.

Notice that the preceding result does not feel the cut locus. To get a result which does, we look at what happens asymptoticly as $T \searrow 0$. What one finds (cf. the first part of Theorem 3.12 in [KS]) is that

$$y \text{ ouside the cut locus of } x \equiv \pi(\mathfrak{e}) \implies \\ \lim_{T \searrow 0} T\big[\nabla \log P_T(\,\cdot\,,y)\big](\geq) = \mathbf{v}(\mathfrak{e},y), \tag{1.3}$$

where $\mathbf{v}(\mathfrak{e}, y)$ is the element of $\mathbb{R}^d$ which is determined by the requirement that the path $\mathfrak{f} \in C^1([0,1]; \mathcal{O}(M))$ satisfying

$$\mathfrak{f}(0) = \mathfrak{e} \text{ and } \dot{\mathfrak{f}}(t) = \mathfrak{E}\big(\mathbf{v}(\mathfrak{e}, y)\big)_{\mathfrak{e}(t)} \tag{1.4}$$

is the horizontal lift to $\mathfrak{e}$ of the (unique) minimal geodesic going from x to y. When y is at the cut locus of x, one should not expect (1.3) to hold. In fact, take $S(x, y)$ in $T_x(M)$ to be the set of initial directions in which minimal geodesics from x to y can proceed. When $S(x, y)$ forms a non-trivial differentiable submanifold, then one can use the second part of Theorem 3.12 in [KS] to see that the limit on the left side of (1.3) exists and is a non-trivial convex combination of elements of $\mathfrak{e}^{-1}\big(S(x, y)\big)$. In particular, since all elements of have the same length, this limit has length strictly less than $\rho(x, y)$ in this case. For example, when M is the circle centered at the origin in $\mathbb{R}^2$ with unit circumference,

$$p_T\left(\theta, \tfrac{1}{2}\right) = (2\pi T)^{-\frac{1}{2}} \sum_{m \in \mathbb{Z}} \exp\left(-\frac{\left(\theta - \frac{1}{2} - m\right)^2}{2T}\right), \tag{1.5}$$

and so it is clear that

$$\lim_{T \searrow 0} T\left[\nabla \log p_T\left(\,\cdot\,, \tfrac{1}{2}\right)\right](0) = 0.$$

The analysis of the Hessian of $\log p_T(\,\cdot\,, y)$ is more challenging. What it leads to is a general estimate (cf. [S]) of the form

$$-\frac{C}{T} \le \big[\text{Hess} \log p_T(\,\cdot\,, y)\big](\mathfrak{e}) \le C\left(\frac{1}{T} + \frac{\rho(x, y)^2}{T^2}\right) \quad \text{for } \mathfrak{e} \in \pi^{-1}(x) \text{ and } (T, x, y) \in (0, 1] \times M^2. \tag{1.6}$$

Unlike the constant in (1.2), the C in (1.6) depends on more than the lower bound α in (1.2). In fact, asymptotic analysis based on [KS] gives

$$y \text{ outside the cut locus of } \implies \lim_{T \searrow 0} T\big[\text{Hess} \log p_T(\,\cdot\,, y)\big](\mathfrak{e}) = -\mathbf{I} + \int_0^1 (1-t)^2 \text{Sec}\big(\mathfrak{f}(t), \mathbf{v}(\mathfrak{e}, y)\big)\, dt, \tag{1.7}$$

where $\mathbf{v}(\mathfrak{e}, y) \in \mathbb{R}^d$ and $\mathfrak{f} \in C^1([0,1]; \mathcal{O}(M))$ are defined as above (cf. (1.4)) and Sec: $\mathcal{O}(M) \times \mathbb{R}^d \longmapsto \mathbb{R}^d \otimes \mathbb{R}^d$ is the (unnormalized) sectional curvature given by

$$\big(\xi, \text{Sec}(\mathfrak{g}, \mathbf{v})\eta\big)_{\mathbb{R}^d} = \big(\text{Riem}_{\mathfrak{g}}(\xi, \mathbf{v})\eta, \mathbf{v}\big)_{\mathbb{R}^d}.$$

On the other hand, when y is at the cut locus of x and the set $S(x, y)$
has the sort of structure described in the preceding paragraph, then one can show that

$$\lim_{T \searrow 0} T^2 \big[\text{Hess} \log p_T(\,\cdot\,, y)\big](\mathfrak{e}) \text{ exists and is strictly positive definite.}$$

For example, in the case of the circle considered above,

$$\lim_{T\searrow 0} T^2 \left[\text{Hess} \log p_T\left(\,\cdot\,,\tfrac{1}{2}\right)\right](0) = \frac{1}{4}.$$

The proofs of these results are based on probabilistic representations of $p_T(\,\cdot\,,y)$ and its derivatives in terms of the Brownian motion on M (cf. (2.2) and (2.12) in [S]).

Remark: Because, by an old result of Varadhan's, one knows that

$$\lim_{T\searrow 0} T \log p_T(x,y) = \frac{\rho(x,y)^2}{2} \text{ for all } x,y \in M,$$

the expression on the right hand side of (1.7) must equal the Hessian of $\frac{1}{2}\rho(\,\cdot\,,y)^2$. However, to date, the author has found no corroboration in differential geometry texts.

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