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AN ESTIMATE ON THE HESSIAN OF THE HEAT KERNEL

DANIEL W. STROOCK

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

$$\mathfrak{E}(\mathbf{v})_{\mathfrak{e}} \in H_{\mathfrak{e}}(\mathcal{O}(M))$$
 and $d\pi \mathfrak{E}(\mathbf{v})_{\mathfrak{e}} = \mathfrak{e}\mathbf{v}$ 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 $\{\mathbf{e}_1,\ldots,\mathbf{e}_d\}$ 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

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

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

$$\nabla F = \sum_{1}^{d} \mathfrak{E}_{k} F \mathbf{e}_{k}, \quad \operatorname{Hess}(F) = \left(\left(\mathfrak{E}_{k} \circ \mathfrak{E}_{\ell} F \right) \right)_{1 \leq k, \ell \leq d}$$

$$\text{and} \quad \Delta F = \sum_{1}^{d} \mathfrak{E}_{k}^{2} F.$$

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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

$$(\nabla f) \circ R_{\mathcal{O}} = \mathcal{O}^{\mathsf{T}} \nabla f$$
, $(\mathrm{Hess}\,(f)) \circ R_{\mathcal{O}} = \mathcal{O}^{\mathsf{T}} \mathrm{Hess}\,(f) \mathcal{O}$, and $(\Delta f) \circ R_{\mathcal{O}} = \Delta f$.

Hence, $|\nabla f|$, $\|\operatorname{Hess}(f)\|_{\operatorname{H.S.}}$ (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

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

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

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

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)

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

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 $T \setminus 0$. What one finds (cf. the first part of Theorem 3.12 in [KS]) is that

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

where $\mathbf{v}(\mathbf{c}, y)$ 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

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

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 $\mathfrak e^{-1}(S(x,y))$. 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,

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

and so it is clear that

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

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

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

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 outside the cut locus of \implies

(1.7)
$$\lim_{T \searrow 0} T \left[\operatorname{Hess} \log p_T(\cdot, y) \right] (\mathfrak{e}) = -\mathbf{I} + \int_0^1 (1 - t)^2 \operatorname{Sec} \left(\mathfrak{f}(t), \mathbf{v}(\mathfrak{e}, y) \right) dt,$$

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

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

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

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

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

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

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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