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GRADIENT ESTIMATES FOR HARMONIC FUNCTIONS ON REGULAR DOMAINS IN RIEMANNIAN MANIFOLDS

ANTON THALMAIER AND FENG-YU WANG

ABSTRACT. Derivative formulae for heat semigroups are used to give gradient estimates for harmonic functions on regular domains in Riemannian manifolds. This probabilistic method provides an alternative to coupling techniques, as introduced by Cranston, and allows to improve some known estimates. We discuss two slightly different ways to exploit derivative formulae where each one should be interesting by itself.

1. INTRODUCTION

Let M be a complete Riemannian manifold of dimension d. Consider the operator $L = \frac{1}{2}(\Delta + Z)$ for some C^1-vector field Z. Choose smooth vector fields $A_1, \dots, A_m$ $(m \geq d)$ and a C^1-vector field A_0 such that

$$L = \tfrac{1}{2} \sum_{i=1}^{m} A_i^2 + A_0 \,. \tag{1.1}$$

Let $A \in \Gamma(\mathbb{R}^m \otimes TM)$ be determined by $A(\,\cdot\,)e_i = A_i$ where $(e_1, \dots, e_m)$ is an orthonormal basis for $\mathbb{R}^m$. We consider the Stratonovich stochastic differential equation

$$\mathrm{d}X = A(X) \circ \mathrm{d}B + A_0(X)\,\mathrm{d}t \tag{1.2}$$

where B is Brownian motion on $\mathbb{R}^m$. There is a (partial) flow $X_t(\,\cdot\,)$ associated to (1.2) such that $X_t(x)$, $0 \leq t < \zeta(x)$, is the maximal solution to (1.2) with starting point $X_0(x) = x$, defined up to the explosion time $\zeta(x)$. Let $V_t = V_t(v) = (T_x X_t)v$ denote the derivative process to $X_t(\,\cdot\,)$ at x in the direction $v \in T_x M$, see [7]; here $T_x X_t\colon T_x M \to T_{X_t(x)} M$ is the differential of $X_t(\,\cdot\,)$ at x. Note that solutions to (1.2) are diffusions on M with generator L.

Let $(P_t u)(x) = \mathbb{E}\big[u\big(X_t(x)\big)\,1_{\{t<\zeta(x)\}}\big]$ be the minimal semigroup to (1.2) acting on bounded measurable functions $u\colon M \to \mathbb{R}$. For $x \in M$, consider the Cameron-Martin space $\mathbb{H}(\mathbb{R}_+, T_x M)$ of absolutely continuous paths $\gamma\colon \mathbb{R}_+ \to T_x M$ such that $|\dot\gamma| \in L^2(\mathrm{d}t)$. Finally, for $x \in M$, let $\mathscr{F}_r(x) = \sigma\big\{X_s(x) : 0 \leq s \leq r\big\}$ be the filtration generated by the solution $X_{\bullet}(x)$ starting from x.

The following theorem is taken from [10] and gives a derivative formula, extending earlier formulae by Elworthy-Li [4]. All these results are centered around Bismut's integration by parts formula [1].

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Theorem 1.1. [10] *Let $u\colon M \to \mathbb{R}$ be bounded measurable, $x \in M$ and $v \in T_xM$. Then, for any bounded $\mathscr{F}_{\bullet}(x)$-adapted process h with sample paths in $\mathbb{H}(\mathbb{R}_+, T_xM)$ such that $\big(\int_0^{\tau_D\wedge t} |\dot h(s)|^2\,\mathrm{d}s\big)^{1/2} \in L^1$, and the property that $h(0)=0$, $h(s)=v$ for all $s \geq \tau_D \wedge t$, the following formula holds:*

$$\langle \nabla P_t u, v\rangle = \mathbb{E}\bigg[u\big(X_t(x)\big)\,1_{\{t<\zeta(x)\}}\int_0^{\tau_D\wedge t}\big\langle (T_xX_s)\,\dot h(s), A\big(X_s(x)\big)\,\mathrm{d}B_s\big\rangle\bigg]. \qquad (1.3)$$

Here τ_D is the first exit time of $X(x)$ from some open neighbourhood D of x such that

$$K_Z = \sup\{-\operatorname{Ric}(w,w) + \langle \nabla_w Z, w\rangle : y \in D,\ w \in T_yM,\ |w|=1\} \qquad (1.4)$$

is finite, and $\|T_xX_r\|\,1_{\{r\leq\tau_D\}} \in L^1$ for each r. Both assumptions on D are satisfied, for instance, if D is relatively compact.

Note that in formula (1.3) the Brownian motion B may live on some high-dimensional $\mathbb{R}^m$; it is known [5] how to reduce the dimension of the Brownian motion to the dimension of the manifold by filtering out redundant noise.

Let τ be an $\mathscr{F}_{\bullet}(x)$-stopping time such that $|(T_xX_r)\,v|\,1_{\{r\leq\tau\}} \in L^1$ for each r. Define a TM-valued process $W(v)$ along $X(x)$ by

$$W_r(v) = \mathbb{E}^{\mathscr{F}_r(x)}\big[(T_xX_r)\,v\,1_{\{r\leq\tau\}}\big] \equiv /\!/_{0,r}\,\mathbb{E}^{\mathscr{F}_r(x)} /\!/_{0,r}^{-1}\,\big[(T_xX_r)\,v\,1_{\{r\leq\tau\}}\big]$$

where $/\!/_{0,r}\colon T_xM \to T_{X_r(x)}M$ denotes parallel transport along $X(x)$. Then $W = W(v)$ satisfies the covariant equation

$$\begin{cases} \dfrac{D}{\partial r}W_r = -\dfrac{1}{2}\big(\operatorname{Ric}(W_r,\,\cdot\,)^{\#} - \nabla_{W_r}Z\big) \\ \quad W_0 = v \end{cases} \qquad (1.5)$$

along $X(x)$ for $r \leq \tau$. Note that, without loss of generality, we may assume that the Levi-Civita connection on M coincides with the Le Jan-Watanabe connection associated to (1.2), see [5]. Further, let

$$\tilde B_r = \int_0^r /\!/_{0,s}^{-1} A\big(X_s(x)\big)\mathrm{d}B_s \qquad (1.6)$$

be the martingale part of the stochastic anti-development of $X(x)$; then $\tilde B$ is a Brownian motion on T_xM, stopped at the lifetime $\zeta(x)$ of $X(x)$; by definition, $A\big(X_s(x)\big)\,\mathrm{d}B_s = /\!/_{0,s}\,\mathrm{d}\tilde B_s$.

Using these notions and given the situation of Theorem 1.1, we have the following analogue to formula (1.3), see [10],

$$\langle \nabla P_t u, v\rangle = \mathbb{E}\bigg[u\big(X_t(x)\big)\,1_{\{t<\zeta(x)\}}\int_0^{\tau_D\wedge t}\big\langle W_s\big(\dot h(s)\big), /\!/_{0,s}\,\mathrm{d}\tilde B_s\big\rangle\bigg], \qquad (1.7)$$

where the process h is as in Theorem 1.1, and D is allowed to be any open neighbourhood D of x such that $K_Z < \infty$. Note that $|W_r(v)| \leq |v|\,\mathrm{e}^{K_Z r/2}$ for $r \leq \tau_D$, as a consequence of the covariant equation (1.5). If K_Z is finite for $D = M$, and $\zeta(x) = \infty$, a.s., then formula (1.7) holds with $\tau_D \equiv \infty$.

For further reference we adopt the above formulae to the case of L-harmonic functions on regular domains. By a regular domain we mean a connected relatively compact subset of M with nonempty smooth boundary.

Theorem 1.2. [10] *Let $D \subset M$ be a regular open domain, $u \in C(\bar{D})$ L-harmonic on D, further $x \in D$ and $v \in T_xM$. Then, for any bounded $\mathscr{F}_{\bullet}(x)$-adapted process h with sample paths in $\mathbb{H}(\mathbb{R}_+, T_xM)$ such that $\big(\int_0^{\tau_D} |\dot{h}(s)|^2 \,\mathrm{d}s\big)^{1/2} \in L^{1+\varepsilon}$ for some $\varepsilon > 0$, and the property that $h(0) = 0$, $h(s) = v$ for all $s \geq \tau_D$, the following formulae hold:*

$$\langle \nabla u(x), v\rangle = \mathbb{E}\Big[\big(u\big(X_{\tau_D}(x)\big) \int_0^{\tau_D} \big\langle (T_xX_s)\,\dot{h}(s), A\big(X_s(x)\big)\,\mathrm{d}B_s\big\rangle\Big], \tag{1.8}$$

and

$$\langle \nabla u(x), v\rangle = \mathbb{E}\Big[\big(u\big(X_{\tau_D}(x)\big) \int_0^{\tau_D} \big\langle W_s\big(\dot{h}(s)\big), //_{0,s}\,\mathrm{d}\tilde{B}_s\big\rangle\Big]. \tag{1.9}$$

The purpose of this paper is to extract gradient estimates for harmonic functions from formula (1.9). Explicit estimates require a proper choice of the process h which turns out to be the main difficulty.

The paper is organized as follows. In Section 3 we use a conformal change of the metric to achieve infinite lifetime of the relevant diffusions on D. The process h in the formulae above can then be chosen deterministically. Section 2 provides the necessary calculations in the new metric. In Section 4 we work directly with (1.9) and construct h via an explicit time change. Although both approaches to gradient estimates are quite similar in nature, the results are not completely comparable. In Section 5 we give explicit local gradient estimates for harmonic functions. Finally, in Section 6, we apply our method to estimate the derivative of heat semigroups.

2. Conformal Change of the Metric

Let $D \subset M$ be a regular open domain with K_Z as in (1.4); note that D is bounded by definition. Next, for $f \in C^2(\bar{D})$ with $f|\partial D = 0$ and $f > 0$ in D, let $L' = f^2L$. We consider the Riemannian metric on D: $\langle\, ,\rangle' = f^{-2}\langle\, ,\rangle$. It is easy to see that

$$\nabla' g = f^2\nabla g, \quad \operatorname{div}' U = \operatorname{div} U - d\cdot f^{-1}Uf, \quad g \in C^1(D),\ U \in \mathscr{X}(D). \tag{2.1}$$

Here $\mathscr{X}(D)$ denotes the set of smooth vector fields on D. Then

$$\begin{aligned} \Delta' &= \operatorname{div}'\nabla' = f^2\Delta - (d-2)f\,\langle \nabla f, \nabla\cdot\rangle, \\ L' &= \frac{1}{2}\big(\Delta' + f^2Z + (d-2)f\,\langle\nabla f, \nabla\cdot\rangle\big). \end{aligned} \tag{2.2}$$

Proposition 2.1. *For $U \in \mathscr{X}(D)$ let $U' = fU$. We have*

$$\begin{aligned} \operatorname{Ric}'(U', U') \geq{}& f^2 \operatorname{Ric}(U,U) + f\Delta f - (d+1)|\nabla f|^2 \\ &+ (d-2)(Uf)^2 + (d-2)f\operatorname{Hess}_f(U,U). \end{aligned} \tag{2.3}$$

Proof. Let $(U_1, \dots, U_d)$ be a local frame normal at x. Let $s = (s_1, \dots, s_d)$ denote normal coordinates around x given by $s = \exp_x \circ\, \iota$ where $\iota = (U_1, \dots, U_d)|_x$ is viewed as isometry from $\mathbb{R}^d$ to T_xM. It suffices to verify (2.3) for $U \in T_xD$ with $|U| = 1$. First, there exists a unit vector $a \in \mathbb{R}^d$ such that $U = \sum_{i=1}^d a_i\,U_i(x)$. Define a function g locally at x by $g \circ s = \sum_{i=1}^d a_is_i$. Then

$$\nabla g(x) = U, \quad \langle \nabla_{U_i}\nabla g, U_i\rangle(x) = \frac{\partial^2}{\partial s_i^2}g(x) = 0. \tag{2.4}$$

By the Weitzenböck formula, we have

$$\mathrm{Ric}'(\nabla' g, \nabla' g) = \frac{1}{2}\Delta' |\nabla' g|'^2 - \langle \nabla' g, \nabla' \Delta' g\rangle' - \|\mathrm{Hess}' g\|'^2. \tag{2.5}$$

Specifically at x,

$$\begin{aligned} \mathrm{Ric}'(U', U') &= f^{-2}\,\mathrm{Ric}'(\nabla' g, \nabla' g) \\ &= \frac{1}{2} f^{-2}\Delta' |\nabla' g|'^2 - f^{-2}\langle \nabla' g, \nabla' \Delta' g\rangle' - f^{-2}\sum_{i=1}^d \langle \nabla'_{U'_i}\nabla' g, U'_i\rangle'^2. \end{aligned} \tag{2.6}$$

Taking into account that $|\nabla' g|' = f|\nabla g|$, $\Delta g(x) = 0$, $\nabla|\nabla g|(x) = 0$ and $|\nabla g|(x) = 1$, we get at the point x:

$$\begin{aligned} f^{-2}\Delta' |\nabla' g|'^2 &= \Delta(f^2|\nabla g|^2) - (d-2)f^{-1}\langle \nabla f, \nabla f^2 |\nabla g|^2\rangle \\ &= f^2\Delta|\nabla g|^2 + 2f\Delta f + 2(3-d)|\nabla f|^2, \end{aligned} \tag{2.7}$$

$$\begin{aligned} f^{-2}\langle \nabla' g, \nabla'\Delta' g\rangle' &= \big\langle \nabla g, \nabla\big[f^2\Delta g - (d-2)f\langle \nabla f, \nabla g\rangle\big]\big\rangle \\ &= f^2\langle \nabla g, \nabla\Delta g\rangle - (d-2)(Uf)^2 - (d-2)f\,\mathrm{Hess}_f(U,U), \end{aligned} \tag{2.8}$$

$$\begin{aligned} f^{-2}\sum_{i=1}^d \langle \nabla'_{U'_i}\nabla' g, U'_i\rangle'^2 &= f^{-2}\sum_{i=1}^d \langle \nabla'_{U_i}(f^2\nabla g), U_i\rangle^2 \\ &= 4\sum_{i=1}^d (U_i f)^2(U_i g)^2 \le 4|\nabla f|^2. \end{aligned} \tag{2.9}$$

Combining equations (2.6) – (2.9), and by using Weitzenböck's formula once again, we obtain (2.3). $\square$

Corollary 2.2. *Let $\tilde Z = f^2 Z + (d-2)f\nabla f$. For any $U \in TD$ with $|U| = 1$, we have*

$$\begin{aligned} &-\mathrm{Ric}'(U', U') + \langle \nabla'_{U'}\tilde Z, U'\rangle' \\ &\qquad \le f^2\big[-\mathrm{Ric}(U,U) + \langle \nabla_U Z, U\rangle\big] + 3\,|\nabla f|^2 + f\,|\nabla f|\,|Z| - f\Delta f. \end{aligned} \tag{2.10}$$

Proof. Extend $U \in TD$ to a vector field on D. Note that for vector fields U, V one has

$$\langle \nabla_U V, U\rangle = \frac{1}{2} V|U|^2 + \langle U, [U,V]\rangle.$$

Thus, we get

$$\begin{aligned} I &:= \langle \nabla'_{U'}\big(f^2 Z + (d-2)\,f\nabla f\big), U'\rangle' \\ &= \frac{1}{2}\big(f^2 Z + (d-2)\,f\nabla f\big)\,|U|^2 + \big\langle U', [U', f^2 Z + (d-2)f\nabla f]\big\rangle' \\ &= \frac{1}{2}\big(f^2 Z + (d-2)f\nabla f\big)|U|^2 + \big\langle U, [U, f^2 Z + (d-2)f\nabla f]\big\rangle - \big(fZ + (d-2)\nabla f\big)f \\ &= \big\langle \nabla_U\big(f^2 Z + (d-2)\,f\nabla f\big), U\big\rangle - fZf - (d-2)\,|\nabla f|^2 \\ &= f^2\langle \nabla_U Z, U\rangle + 2f(Uf)\langle Z, U\rangle - fZf + (d-2)\big[(Uf)^2 + f\,\mathrm{Hess}_f(U,U) - |\nabla f|^2\big]. \end{aligned}$$

Let $Z_0 = Z - \langle Z, U\rangle U$, then $|\langle Z, U\rangle U - Z_0| = |Z|$, and

$$2f(Uf)\langle Z, U\rangle - fZf = f\big(\langle Z, U\rangle U - Z_0\big)f \le f\,|\nabla f|\,|Z|.$$

Therefore,

$$I \le f^2\langle \nabla_U Z, U\rangle + f\,|\nabla f|\,|Z| + (d-2)\big[(Uf)^2 + f\operatorname{Hess}_f(U,U) - |\nabla f|^2\big].$$

Combining this and (2.3), we get the estimate (2.10). □

By (2.2), we have $2L' = \Delta' + \tilde Z$. Hence, any L'-diffusion process is a Brownian motion with drift on the Riemannian manifold $(D, \langle\,,\,\rangle')$. The following result says that the lifetime of such diffusions is infinite.

Proposition 2.3. *Let X be an L'-diffusion process on a regular open domain D with $X_0 = x \in D$ and lifetime $\tau = \inf\{t \ge 0 : X_t \in \partial D\}$. Then $\tau = \infty$, a.s.*

Proof. For $n \ge 1$, let $\tau_n = \inf\{t \ge 0 : f(X_t) \le 1/n\}$. For $x \in D$, choose $n_0 \ge 1$ such that $f(x) \ge 1/n_0$. Note that $L' f^{-1} = -Lf + f^{-1}|\nabla f|^2 \le cf^{-1}$ for some constant c. Then

$$\mathbb{E} f^{-1}(X_{t\wedge\tau_n}) \le f^{-1}(x)\,\mathrm{e}^{ct}, \quad t \ge 0,\ n \ge n_0.$$

But $\mathbb{E} f^{-1}(X_{t\wedge\tau_n}) \ge n\,\mathbb{P}\{\tau_n < t\}$, hence

$$\mathbb{P}\{\tau_n < t\} \le n^{-1} f^{-1}(x)\,\mathrm{e}^{ct}.$$

So $\mathbb{P}\{\tau < t\} = 0$, $t \ge 0$. This proves the proposition. □

3. Gradient Estimates (First Method)

Let $D \subset M$ be an open regular domain. As above, let $f \in C^2(\bar D)$ with $f|\partial D = 0$ and $f > 0$ in D. Rewrite $L' = f^2 L$ as $L' = \frac{1}{2}\sum_{i=1}^{\ell} A_i^2 + A_0$ for some $A_i \in \mathscr{X}(D)$ and a C^1-vector field A_0. Consider the equation

$$\mathrm{d}X_t = A(X_t)\circ \mathrm{d}B_t + A_0(X_t)\,\mathrm{d}t \tag{3.1}$$

where B is a Brownian motion on $\mathbb{R}^\ell$ and $A(\,\cdot\,)e_i = A_i$ as in Section 1. Then solutions to (3.1) are L'-diffusion processes. Thus, from Theorem 1.1, (1.7) and (2.10), we derive the following special case where h is non-random.

Corollary 3.1. *Let $(P'_t u)(x) = \mathbb{E}\big[u(X_t(x))\big]$ be the semigroup of L'. For any bounded measurable function u on D and $h \in \mathbb{H}([0,t],\mathbb{R})$ with $h(0) = 0$, $h(t) = 1$, we have*

$$\langle \nabla' P'_t u, v\rangle' = \mathbb{E}\left[u\big(X_t(x)\big)\int_0^t \big\langle \dot h(s)\,W_s(v), /\!/_{0,s}\,\mathrm{d}\tilde B_s\big\rangle'\right], \quad x \in D,\ v \in T_x D. \tag{3.2}$$

Here $\tilde B$ is a Brownian motion on $T_x M$. Note that $/\!/_{0,s}$ corresponds to parallel transport on D along $X_\bullet(x)$ with respect to the new metric $\langle\,,\,\rangle'$. According to (1.5), since $L' = \frac{1}{2}(\Delta' + \tilde Z)$, the process $W_r(v)$ solves the following covariant equation along $X_r(x)$:

$$\frac{D}{\partial r} W_r(v) = -\frac{1}{2}\Big(\operatorname{Ric}'(W_r(v),\,\cdot\,)^{\#} - \nabla'_{W_r(v)}\tilde Z\Big), \quad W_0(v) = v.$$

Now, with the help of (3.2), we are ready to turn to gradient estimates for L-harmonic functions.

Theorem 3.2. *Let $D \subset M$ be an open regular domain. For some $f \in C^2(\bar D)$ with $f|\partial D = 0$ and $f > 0$ in D, let*

$$c(f) = \sup_D \Big\{ f^2 K_Z + 3\,|\nabla f|^2 + f|\nabla f|\,|Z| - f\Delta f \Big\}. \tag{3.3}$$

If u is a bounded positive L-harmonic function on D, then

$$|\nabla u(x)| \le \frac{1}{f(x)} \sqrt{c(f)\, u(x)\, \|u\|_D}, \tag{3.4}$$

$$|\nabla u(x)| \le \frac{\|u\|_D}{f(x)} \sqrt{\frac{c(f)}{2\pi}}\, \inf_{r>0} \frac{r}{1-\mathrm{e}^{-r^2/2}}. \tag{3.5}$$

Proof. It is easy to see that $c(f) \ge 0$. For any $\varepsilon > 0$, let $c_\varepsilon = c(f) + \varepsilon$. For $v \in T_xD$, we have $|W_s(v)|' \le |v|'\,\mathrm{e}^{c_\varepsilon s/2}$. Take

$$h(s) = \frac{c_\varepsilon \delta}{1-\mathrm{e}^{-c_\varepsilon \delta t}} \int_0^s \mathrm{e}^{-c_\varepsilon \delta r}\,\mathrm{d}r, \ \ s \in [0,t], \ \ \delta > \frac{1}{2},$$

then $R_t = \int_0^t \langle \dot h(s)\, W_s(v), //_{0,s}\, \mathrm{d}\tilde B_s\rangle'$ is an L^2-martingale. Noting that $P_t' u \equiv u$, $t \ge 0$, we obtain from Corollary 3.1

$$|\nabla u(x)| = f^{-1}(x)\,|\nabla' u(x)|' \le f^{-1}(x) (P_t' u^2(x))^{1/2} (\mathbb{E}\, R_t^2)^{1/2}, \quad t \ge 0, \tag{3.6}$$

for some $|v|' \le 1$. Thus, in explicit terms,

$$\mathbb{E}\, R_t^2 = \int_0^t \mathrm{e}^{c_\varepsilon s}\, \dot h(s)^2\,\mathrm{d}s = \int_0^t \frac{c_\varepsilon^2\, \delta^2}{(1-\mathrm{e}^{-c_\varepsilon \delta t})^2}\, \mathrm{e}^{(1-2\delta)c_\varepsilon s}\,\mathrm{d}s,$$

and therefore,

$$\mathbb{E}\, R_t^2 = \frac{c_\varepsilon\, \delta^2 (1-\mathrm{e}^{-c_\varepsilon(2\delta-1)t})}{(2\delta-1)(1-\mathrm{e}^{-c_\varepsilon \delta t})^2}. \tag{3.7}$$

By this and (3.6), letting $t \to \infty$, we obtain

$$|\nabla u| \le f^{-1} \sqrt{u\, \|u\|_D\, c_\varepsilon}\, \inf_{\delta > 1/2} \frac{\delta}{\sqrt{2\delta - 1}} = f^{-1}\sqrt{u\,\|u\|_D\, c_\varepsilon}.$$

This proves (3.4) by letting $\varepsilon \to 0$.

Next, for the proof of (3.5), let

$$b_t = \int_0^t \frac{1}{|W_s(v)\, \dot h(s)|'} \big\langle W_s(v)\, \dot h(s), //_{0,s}\, \mathrm{d}\tilde B_s \big\rangle'. \tag{3.8}$$

Note that $W_s(v) \ne 0$, a.s., and $\dot h > 0$ by definition. Since $[b_t, b_t] = t$ for the quadratic variation, (3.8) defines a Brownian motion, consequently $\mathbb{E}\,|b_t| = \sqrt{2t/\pi}$. By Corollary 3.1 we obtain

$$|\nabla u| \le f^{-1} \|u\|_D \sqrt{2/\pi}\, c_\varepsilon \inf_{\delta > 1/2,\, t > 0}\ \sup_{s \in [0,t]} \frac{\sqrt{t}\, \delta\, \mathrm{e}^{c_\varepsilon(\delta - 1/2)s}}{1-\mathrm{e}^{-c_\varepsilon \delta t}}.$$

Now, (3.5) follows from the choice $\delta \to 1/2$ and $\varepsilon \to 0$. □

Theorem 3.2 provides general formulae for gradient estimates of harmonic functions on regular domains. For each f, there is an upper bound. In Section 5, we give examples for the choice of f.

4. Gradient Estimates (Second Method)

Now we are going to introduce a slightly different approach to gradient estimates for L-harmonic functions. Let f and D be as in Section 3, and $L = \frac{1}{2}(\Delta + Z)$. We represent L according to (1.1) and construct L-diffusions by solving the SDE (1.2). We may restrict ourselves to L-diffusions on D with lifetime τ_D (exit time from D). For $x \in D$, consider the strictly increasing process

$$T(t) = \int_0^t f^{-2}\big(X_s(x)\big)\mathrm{d}s, \quad t \le \tau_D,$$

and

$$\tau(t) = \inf\{s \ge 0 : T(s) \ge t\}.$$

Obviously $T\big(\tau(t)\big) = t$ since $\tau_D < \infty$, and $\tau\big(T(t)\big) = t$ for $t \le \tau_D$. Note that, since X is a diffusion with generator L, the time-changed diffusion $X'_t = X_{\tau(t)}$ has generator $L' = f^2 L$. In particular, the lifetime $T(\tau_D)$ of X' is infinite by Proposition 2.3.

Let $u \in C(\bar{D})$ be L-harmonic on D. In this section, we work directly with formula (1.9). To this end, fix $t > 0$ and let

$$h_0(s) = \int_0^s f^{-2}\big(X_r(x)\big)\, 1_{\{r<\tau(t)\}}\mathrm{d}r, \quad s \ge 0.$$

Then, for $s \ge \tau(t)$,

$$h_0(s) = h_0\big(\tau(t)\big) = \int_0^{\tau(t)} f^{-2}\big(X_r(x)\big)\,\mathrm{d}r = t.$$

Next, let $h_1 \in C^1([0,t],\mathbb{R})$ with $h_1(0) = 0$, $h_1(t) = t$. Take $h(s) = t^{-1}v\,(h_1 \circ h_0)(s)$ where v is a tangent vector in T_xM. Then h is an adapted bounded process with $h(0) = 0$, $h(s) = v$ for $s \ge \tau(t)$. Thus, according to Theorem 1.2,

$$\begin{aligned}\big\langle \nabla u(x), v\big\rangle &= \frac{1}{t}\mathbb{E}\Big[u\big(X_{\tau_D}(x)\big)\int_0^{\tau(t)} (\dot{h}_1 \circ h_0)(s)\big\langle f^{-2}\big(X_s(x)\big)T_xX_s v, A\big(X_s(x)\big)\mathrm{d}B_s\big\rangle\Big] \\ &= \frac{1}{t}\mathbb{E}\Big[u\big(X_{\tau_D}(x)\big)\int_0^{\tau(t)} (\dot{h}_1 \circ h_0)(s)\big\langle f^{-2}\big(X_s(x)\big)W_s(v), /\!/_{0,s}\,\mathrm{d}\tilde{B}_s\big\rangle\Big].\end{aligned} \tag{4.1}$$

It remains to show that $\big(\int_0^{\tau(t)} |\dot{h}(s)|^2\,\mathrm{d}s\big)^{1/2} \in L^{1+\varepsilon}$ for some $\varepsilon > 0$. For instance, we may take $\varepsilon = 1$. Obviously, with $c_1 = \sup_{[0,t]}|\dot{h}_1|^2$, we have

$$\begin{aligned}\int_0^{\tau(t)} |\dot{h}(s)|^2\,\mathrm{d}s &\le c_1|v|^2\frac{1}{t^2}\int_0^{\tau(t)} f^{-4}\big(X_s(x)\big)\,\mathrm{d}s \\ &= c_1|v|^2\frac{1}{t^2}\int_0^{\tau(t)} f^{-2}\big(X_s(x)\big)\,\mathrm{d}T(s) \\ &= c_1|v|^2\frac{1}{t^2}\int_0^{t} f^{-2}\big(X_{\tau(s)}(x)\big)\,\mathrm{d}s.\end{aligned}$$

On the other hand, we know that $\mathrm{d}\,f^{-2}(X_{\tau(s)}) = \mathrm{d}\,f^{-2}(X'_s)$ and

$$L'f^{-2} = f^2Lf^{-2} = f^2\big(3\,f^{-4}|\nabla f|^2 - 2\,f^{-3}Lf\big) \le c_2 f^{-2} \tag{4.2}$$

with a constant $c_2 > 0$. Let $\sigma_n = \inf\{t \geq 0 : f^{-2}(X'_t) \geq n\}$, by Itô's formula and Gronwall's lemma, we obtain

$$\mathbb{E} f^{-2}(X'_{s\wedge\sigma_n}) \leq f^{-2}(x)\,\mathrm{e}^{c_2 s}$$

for $f^{-2}(x) < n$. Hence, by Fatou's lemma,

$$\mathbb{E} f^{-2}(X'_s) = \mathbb{E} \lim_{n\to\infty} f^{-2}(X'_{s\wedge\sigma_n}) \leq \varliminf_{n\to\infty} \mathbb{E} f^{-2}(X'_{s\wedge\sigma_n}) \leq f^{-2}(x)\,\mathrm{e}^{c_2 s},$$

and consequently, $\mathbb{E}\Big[\int_0^{\tau(t)} f^{-4}(X_s)\,\mathrm{d}s\Big] = \mathbb{E}\Big[\int_0^t f^{-2}(X_{\tau(s)})\,\mathrm{d}s\Big] < \infty$.

From Equation (4.1) we obtain the following result, similar to estimate (3.4) in Theorem 3.2.

Theorem 4.1. *Let $D \subset M$ be a regular open domain. Given f as above, let*

$$c_1(f) = \sup_D \Big\{ f^2 K_Z^+ + 3\,|\nabla f|^2 - f(\Delta + Z)f \Big\}. \tag{4.3}$$

For any bounded positive L-harmonic function u on D, we have

$$|\nabla u| \leq \frac{1}{f}\sqrt{u\,\|u\|_D\, c_1(f)}. \tag{4.4}$$

Proof. As in the proof of Theorem 3.2 we may assume $c_1(f) > 0$; otherwise we add $\varepsilon > 0$ and take the limit as $\varepsilon \to 0$ at the end.

Let $|v| = 1$ and $R_s = \int_0^s (\dot{h}_1 \circ h_0)(s)\,\big\langle f^{-2}\big(X_r(x)\big)\,W_r(v), //_{0,r}\,\mathrm{d}\tilde{B}_r\big\rangle$, $s \leq \tau(t)$. Note that $|W_s(v)| \leq \mathrm{e}^{K_Z s/2}$. From this we conclude

$$\mathrm{d}R_s^2 \leq 2R_s\,\mathrm{d}R_s + (\dot{h}_1 \circ h_0)^2(s)\, f^{-4}(X_s)\,\mathrm{e}^{K_Z s}\mathrm{d}s, \quad s \leq \tau(t).$$

Recall that $h_0(\tau(s)) = s \wedge t$, thus we obtain

$$\mathbb{E} R_{\tau(t)}^2 \leq \mathbb{E}\int_0^{\tau(t)} (\dot{h}_1 \circ h_0)^2(s)\, f^{-4}(X_s)\,\mathrm{e}^{K_Z s}\mathrm{d}s = \int_0^t \dot{h}_1(s)^2\,\mathbb{E} f^{-2}(X'_s)\,\mathrm{e}^{K_Z \tau(s)}\mathrm{d}s.$$

Note that $\mathrm{d}\tau(s) = f^2(X'_s)\,\mathrm{d}s$, so by (4.2) we get

$$\begin{aligned}
\mathrm{d}\big[f^{-2}(X'_s)\mathrm{e}^{K_Z\tau(s)}\big] &= \mathrm{d}M_s + K_Z \mathrm{e}^{K_Z\tau(s)}\mathrm{d}s + (3\,|\nabla f|^2 - 2fLf)\,\mathrm{e}^{K_Z\tau(s)} f^{-2}(X'_s)\,\mathrm{d}s \\
&\leq \mathrm{d}M_s + c_1(f)\,\mathrm{e}^{K_Z\tau(s)} f^{-2}(X'_s)\,\mathrm{d}s
\end{aligned} \tag{4.5}$$

for some local martingale M_s. Consequently, by the argument right before this theorem,

$$\mathbb{E} f^{-2}(X_{\tau(s)})\,\mathrm{e}^{K_Z\tau(s)} \leq f^{-2}(x)\,\mathrm{e}^{c_1(f)s}.$$

Now, taking

$$h_1(s) = \frac{t\,c_1(f)}{1 - \mathrm{e}^{-c_1(f)t}} \int_0^s \mathrm{e}^{-c_1(f)r}\mathrm{d}r,$$

we obtain

$$\mathbb{E} R_{\tau(t)}^2 \leq \frac{t^2 c_1(f)^2}{f(x)^2(1 - \mathrm{e}^{-c_1(f)t})^2}\int_0^t \mathrm{e}^{-c_1(f)s}\mathrm{d}s = \frac{t^2 c_1(f)}{f(x)^2(1 - \mathrm{e}^{-c_1(f)t})}.$$

The last estimate together with (4.1) gives

$$|\nabla u| \leq \frac{1}{t}\sqrt{u\,\|u\|_D\,\mathbb{E} R_{\tau(t)}^2} \leq \frac{\sqrt{u\,\|u\|_D\, c_1(f)}}{f\sqrt{1 - \mathrm{e}^{-c_1(f)t}}}.$$

The desired result follows by letting $t \to \infty$. $\square$

5. Explicit Upper Bounds

In this section we put the general estimates of Theorem 3.2 and Theorem 4.1 in concrete form by giving examples for appropriate functions f and calculating the corresponding upper bounds.

Corollary 5.1. *Let $D \subset M$ be a regular open domain, $L = \frac{1}{2}(\Delta + Z)$ for some C^1-vector field Z on M. Let $b = \|Z\|_D := \sup_D |Z|$. For $x \in D$, let $\delta_x = \rho(x, \partial D)$ where ρ denotes the Riemannian distance. Further, let*

$$C(r) = \sqrt{\pi^2(d+3)r^{-2} + 2\pi\Big(b + \sqrt{K_0^+(d-1)}\Big)r^{-1} + 4K_Z^+}\,. \tag{5.1}$$

For a bounded positive L-harmonic function u on D, we have

$$|\nabla u(x)| \le \frac{1}{2}\sqrt{u(x)\,\|u\|_D}\,C\big(\delta_x\big), \tag{5.2}$$

$$|\nabla u(x)| \le \|u\|_D\,\frac{1}{2\sqrt{2\pi}}\,C\big(\delta_x\big)\inf_{r>0}\frac{r}{1-\mathrm{e}^{-r^2/2}}\,. \tag{5.3}$$

If $D = M$ and M noncompact without boundary, then

$$|\nabla u| \le \sqrt{u\,\|u\|_\infty K_Z^+}, \tag{5.4}$$

$$|\nabla u| \le \frac{\|u\|_\infty}{\sqrt{2\pi}}\sqrt{K_Z^+}\,\inf_{r>0}\frac{r}{1-\mathrm{e}^{-r^2/2}}\,. \tag{5.5}$$

Proof. 1) We fix $x \in D$ and let $\bar\delta_x = \delta_x \wedge \iota_x$ where $\iota_x = \rho(x, \mathrm{cut}(x))$. Further, let $B = B(x, \bar\delta_x)$ denote the open ball about x of radius $\bar\delta_x$. Then, Theorems 3.2 and 4.1 hold with D replaced by B. Take $f(p) = \cos\big(\pi\rho(x,p)/(2\bar\delta_x)\big) = \bar f(\rho(x,p))$ where ρ is the Riemannian distance. Obviously, $|f| \le 1$, $f(x) = 1$, $\|\nabla f\|_B = \pi/(2\bar\delta_x)$. Next, for $p \in D$, we have

$$\Delta\rho(x,\cdot\,)(p) \le \sqrt{(d-1)K_0^+}\coth\Big(\sqrt{K_0^+/(d-1)}\,\rho(x,p)\Big),$$

and hence, with $\rho = \rho(x,\cdot\,)$,

$$-\Delta f \le \frac{\pi\sqrt{K_0^+(d-1)}}{2\bar\delta_x}\sin\Big(\frac{\pi\rho}{2\bar\delta_x}\Big)\coth\Big(\sqrt{K_0^+/(d-1)}\,\rho\Big) + \frac{\pi^2}{4\bar\delta_x^2}\cos\Big(\frac{\pi\rho}{2\bar\delta_x}\Big).$$

It is easy to see that $\coth r \le 1 + r^{-1}$, $r > 0$. Thus

$$\sin\Big(\frac{\pi\rho}{2\bar\delta_x}\Big)\coth\Big(\sqrt{K_0^+/(d-1)}\,\rho\Big) \le 1 + \frac{\pi\sqrt{d-1}}{2\bar\delta_x\sqrt{K_0^+}}\,.$$

Hence

$$-\Delta f \le \frac{\pi\sqrt{K_0^+(d-1)}}{2\bar\delta_x} + \frac{\pi^2 d}{4\bar\delta_x^2}\,.$$

Therefore,

$$c(f) \le K_Z^+ + \frac{\pi^2(d+3)}{4\bar{\delta}_x^2} + \frac{\pi\big(b+\sqrt{K_0^+(d-1)}\big)}{2\bar{\delta}_x},$$

the same is true for $c_1(f)$. Now, by Theorem 3.2 or Theorem 4.1, this proves (5.2) and (5.3) with $\bar{\delta}_x$ instead of δ_x on the right-hand side.

2) We want to show that $\bar{\delta}_x = \delta_x \wedge \iota_x$ may be replaced by δ_x in 1) and the estimates do not depend on ι_x. According to [6], we have

$$\mathrm{d}\rho(x, X_t) = \mathrm{d}b_t + L\rho(x, X_t)\,\mathrm{d}t - \mathrm{d}\ell_t,$$

where b_t is a one-dimensional Brownian motion and ℓ_t is an increasing process with support contained in $\{t \ge 0 : X_t \in \mathrm{cut}(x)\}$, i.e., $1_{\{t:\, X_t \notin \mathrm{cut}(x)\}}\,\mathrm{d}\ell_t = 0$, a.s. (Here $L\rho(x,\cdot) = 0$ at points where $\rho(x,\cdot)$ is not differentiable.) Then, for the choice of $f(p) = \cos\big(\frac{\pi}{2\delta_x}\rho(x,p)\big)$, we have

$$\mathrm{d}f^{-2}(X_{\tau(s)}) \equiv \mathrm{d}\,f^{-2}(X_s') \le \mathrm{d}M_t + L'f^{-2}(X_s')\,\mathrm{d}s.$$

This means that all the arguments in the proofs of formula (4.1) and Theorem 4.1 remain valid for the present f.

3) When $D = M$, by [10], one may take $f \equiv 1$ in Corollary 3.1, then (5.4) and (5.5) follow. □

Corollary 5.2. *Let $D = B(p,R)$, $x \in D$. For a bounded positive L-harmonic function u on D, we have*

$$|\nabla u(x)| \le \frac{\sqrt{u(x)\,\|u\|_D}}{2\sin(\pi\delta_x/(2R))}\,C(R),$$

$$|\nabla u(x)| \le \frac{\|u\|_D}{2\sqrt{2\pi}\sin(\pi\delta_x/(2R))}\,C(R)\inf_{r>0}\frac{r}{1-\mathrm{e}^{-r^2/2}}$$

with $\delta_x = \rho(x,\partial D)$ and $C(R)$ given by (5.1).

Proof. Choose $f(x) = \sin(\pi\delta_x/(2R))$, then the proof is similar to that of Corollary 5.1. □

Remarks. 1) Gradient estimates in global form, that is, for positive harmonic functions defined on complete manifolds, have been proved by S. T. Yau [14]. Local versions are due to Cheng and Yau [2], and more generally, for positive solutions of the heat equation, to Li and Yau [8], e.g., Theorem 1.2, p. 158. See also the lectures of R. Schoen [9] for a survey on the analytic method where a gradient estimate for positive harmonic functions on geodesic balls is presented.

2) As far as we know, for the domain case, there are rarely explicit estimates as given above. One may also refer to Cranston's paper [3] and references therein. For elliptic operators on $\mathbb{R}^d$, there are some explicit estimates for this case (see [12]). For regular domains, an estimate is presented in [13] (using coupling):

$$|\nabla u| \le 2d\mathrm{e}\max\Big\{\sqrt{K_0^+(d-1)} + 2b,\, \delta_x^{-1}\Big\}\|u\|_D$$

which does not depend on K_Z. But, for small δ_x, it is not as good as Corollary 5.1.

3) Even in the case $D = M$, the estimate in Corollary 5.1 is new, but for the case $Z = 0$, there is a slightly better one given in [11] (using coupling):

$$|\nabla u| \le \sqrt{K_0^+(d-1)}\,\Big\{\sqrt{2\pi(d-1)} + \mathrm{e}^{1-d}\Big\}^{-1}\|u\|_\infty \le \sqrt{\frac{K_0^+}{2\pi}}\,\|u\|_\infty.$$

6. Gradient Estimates for Heat Semigroups

Finally, we consider gradient estimates of (not necessarily conservative) heat semigroups. Let

$$(P_t u)(x) = \mathbb{E}\big[u\big(X_t(x)\big)1_{\{t<\zeta(x)\}}\big] \tag{6.1}$$

where ζ is the lifetime of the process. By virtue of formula (1.7), we have for $x \in D$ and $v \in T_xM$

$$\langle \nabla P_t u, v\rangle = \mathbb{E}\left[u\big(X_t(x)\big)\, 1_{\{t<\zeta(x)\}} \int_0^{\tau_D\wedge t} \big\langle W_s(\dot h(s)), //_{0,s}\, \mathrm{d}\tilde B_s\big\rangle\right], \tag{6.2}$$

where D is any open regular domain such that $x \in D$, h a bounded adapted process with sample paths in $\mathbb{H}(\mathbb{R}_+, T_xM)$ such that $h(0) = 0$, $h(s) = v$ for $s \geq \tau_D \wedge t$, and $(\int_0^{t\wedge\tau_D} \|\dot h\|^2)^{1/2} \in L^1$.

In the sequel we assume $\|f\|_D \leq 1$ which implies $\tau(s) \leq s$. We take h_0, h_1 as above, and set $h = (h_1 \circ h_0)\, v/t$. Then

$$\langle \nabla P_t u, v\rangle = \frac{1}{t}\mathbb{E}\left[u(X_t)1_{\{t<\zeta\}} \int_0^{\tau(t)} (\dot h_1 \circ h_0)(s)\, \big\langle f^{-2}(X_s)\, W_s(v), //_{0,s}\, \mathrm{d}\tilde B_s\big\rangle\right]. \tag{6.3}$$

From this formula and the same arguments as in the proofs of Theorem 4.1 and Corollary 5.2, we get the following result.

Theorem 6.1. *Let $D \subset M$ be an open regular domain, $f \in C^2(\bar D)$ with $f|\partial D = 0$, $f > 0$ in D and $\|f\|_D \leq 1$. For any bounded positive measurable function u: $M \to \mathbb{R}$ and $t > 0$, we have the following estimate on D where $c_1(f)$ is given by (4.3):*

$$|\nabla P_t u| \leq \frac{\sqrt{\|u\|_\infty\, c_1(f) P_t u}}{f\sqrt{1-\mathrm{e}^{-c_1(f)t}}}. \tag{6.4}$$

In particular, for $D = B(x,R)$ and $C(R)$ defined by (5.1), we have

$$|\nabla P_t u(x)| \leq \frac{C(R)\sqrt{\|u\|_\infty P_t u(x)}}{2\sqrt{1-\mathrm{e}^{-C(R)^2t/4}}}. \tag{6.5}$$

Remarks. 1) For $0 < s < t$, we may write $P_t u = P_s(P_{t-s}u)$. Taking this into account, we obtain

$$|\nabla P_t u| \leq \frac{\sqrt{\|P_{t-s}u\|_\infty c_1(f) P_t u}}{f\sqrt{1-\mathrm{e}^{-c_1(f)s}}}.$$

2) One may also consider the minimal semigroup on D:

$$(P_t^D u)(x) = \mathbb{E}\big[u\big(X_t(x)\big)1_{\{t<\tau_D\}}\big]. \tag{6.6}$$

In this case, Theorem 6.1 holds for P_t^D with $\|u\|_\infty$ replaced by $\|u\|_D$.

We also like to remark that Theorem 6.1 can be used to estimate the gradient of the heat kernel. For instance, let p_t: $M \times M \to \mathbb{R}_+$ $(t > 0)$ be the smooth heat kernel associated to (6.1),

$$(P_t u)(x) = \mathbb{E}\big[u\big(X_t(x)\big)\, 1_{\{t<\zeta(x)\}}\big] = \int_M p_t(x,y)\, u(y)\, \mathrm{vol}(dy).$$

Then $(P_s u)(x) = p_t(x,y)$ for $u = p_{t-s}(\,\cdot\,,y)$, $0 < s < t$. Hence, from (6.4) we get as special case the following result.

Corollary 6.2. *On any open regular domain $D \subset M$ we have*

$$\left|\nabla\sqrt{p_t(\,\cdot\,,y)}\right| \le \frac{\sqrt{\|p_{t-s}(\,\cdot\,,y)\|_\infty\, c_1(f)}}{2f\sqrt{1-e^{-c_1(f)s}}}\,,$$

for $0<s<t$ where f is as above with $\|f\|_D \le 1$.

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NWF–I Mathematik, Universität Regensburg, D-93040 Regensburg, Germany
E-mail address: anton.thalmaier@mathematik.uni-regensburg.de

Department of Mathematics, Beijing Normal University, Beijing 100875, China
E-mail address: wangfy@bnu.edu.cn