Li-Yau Type Gradient Estimates and Harnack Inequalities by Stochastic Analysis

Marc Arnaudon, Anton Thalmaier

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Abstract.

In this paper we use methods from Stochastic Analysis to establish Li-Yau type estimates for positive solutions of the heat equation. In particular, we want to emphasize that Stochastic Analysis provides natural tools to derive local estimates in the sense that the gradient bound at given point depends only on universal constants and the geometry of the Riemannian manifold locally about this point.

§1. Introduction

The effect of curvature on the behaviour of the heat flow on a Riemannian manifold is a classical problem. Ricci curvature manifests itself most directly in gradient formulas for solutions of heat equation.

Gradient estimates for positive solutions of the heat equation serve as infinitesimal versions of Harnack inequalities: by integrating along curves on the manifold local gradient estimates may be turned into local Harnack type inequalities.

Solutions to the heat equation

$$\frac{\partial}{\partial t}u = \frac{1}{2}\,\Delta u \tag{1.1}$$

on a Riemannian manifold M are well understood in probabilistic terms. For instance, if $u = u(x,t)$ denotes the minimal solution to (1.1), then a straightforward calculation using Itô's calculus leads to the stochastic representation of u as

$$u(x,t) = \mathbb{E}\left[1_{\{t<\zeta(x)\}}\, f(X_t(x))\right] \tag{1.2}$$

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where $f = u(\cdot, 0)$ is the initial condition in (1.1), $X_\bullet(x)$ denotes a Brownian motion on M, starting from x at time 0, and $\zeta(x)$ its lifetime.

It is a remarkable fact that exact stochastic representation formulas for the derivative of solutions to the heat equation can be given, expressing the gradient ∇u of u in terms of Ricci curvature.

The following typical example for such a Bismut type derivative formula is taken from [11].

Theorem 1.1 (Stochastic representation of the gradient)**.** *Let D be a relatively compact open domain in a complete Riemannian manifold M, and let $u = u(x,t)$ be a solution of the heat equation* (1.1) *on $D \times [0,T]$ which is continuous on $\bar{D} \times [0,T]$. Then, for any $v \in T_xM$ and $x \in D$,*

$$\langle \nabla u(\cdot, T)_x, v\rangle = -\mathbb{E}\left[u(X_\tau(x), T-\tau)\int_0^\tau \left\langle Q_s\,\dot{\ell}_s, dB_s\right\rangle\right], \tag{1.3}$$

where:

(1) *$X \equiv X_\bullet(x)$ is a Brownian motion on M, starting at x, and $\tau = \tau(x) \wedge T$ where*

$$\tau(x) = \inf\{t > 0 : X_t(x) \notin D\}$$

is the first exit time from D; the stochastic integral is taken with respect to the Brownian motion B in T_xM, related to X by the Stratonovich equation $dB_t = /\!/_t^{-1}\delta X_t$, where $/\!/_t : T_xM \to T_{X_t}M$ denotes the stochastic parallel transport along X.

(2) *The process Q takes values in the group of linear automorphisms of T_xM and is defined by the pathwise covariant ordinary differential equation,*

$$dQ_t = -\tfrac{1}{2}\,\mathrm{Ric}_{/\!/_t}(Q_t)\,dt, \quad Q_0 = \mathrm{id}_{T_xM},$$

where $\mathrm{Ric}_{/\!/_t} = /\!/_t^{-1} \circ \mathrm{Ric}^\sharp_{X_t} \circ /\!/_t$ (a linear transformation of T_xM), and $\langle \mathrm{Ric}^\sharp_z\, u, w\rangle = \mathrm{Ric}_z(u,w)$ for any $u, w \in T_zM$, $z \in M$.

(3) *Finally, ℓ_t may be any adapted finite energy process taking values in T_xM such that $\ell_0 = v$, $\ell_\tau = 0$ and*

$$\Big(\int_0^\tau |\dot{\ell}_t|^2\,dt\Big)^{1/2} \in L^{1+\varepsilon} \quad \text{for some } \varepsilon > 0.$$

Formula (1.3) is valid for any solution u of the heat equation and does not require positivity of u.

Remark 1.2. Formula (1.3) is easily adapted to more specific situations, for instance:

(i) Let $u = u(x,t)$ be a solution of the heat equation (1.1) on $D \times [0,T]$ such that $u|_{t=0} = f$ and $u(\cdot,t)|\partial D = f|\partial D$. Then

$$\langle \nabla u(\cdot,T)_x, v\rangle = -\mathbb{E}\left[f(X_\tau(x)) \int_0^\tau \left\langle Q_s\, \dot{\ell}_s, dB_s\right\rangle\right], \quad \tau = \tau(x) \wedge T\,.$$

(ii) Let $u = u(x,t)$ be a solution of the heat equation (1.1) on $D \times [0,T]$ such that $u|_{t=0} = f$ and $u(\cdot,t)|\partial D = 0$. Then

$$\langle \nabla u(\cdot,T)_x, v\rangle = -\mathbb{E}\left[f(X_T(x))\, 1_{\{T<\tau(x)\}} \int_0^{\tau(x)\wedge T} \left\langle Q_s\, \dot{\ell}_s, dB_s\right\rangle\right].$$

Such formulas are interesting by several means. For instance, on a complete Riemannian manifold M, starting from the minimal solution to the heat equation

$$u(x,T) = \mathbb{E}\left[1_{\{T<\zeta(x)\}}\, f(X_T(x))\right] \tag{1.4}$$

with bounded initial conditions $u(\cdot,0) = f$, since for arbitrarily small $T > 0$ Brownian motion explores the whole manifold M, we observe that the global structure of M enters in formula (1.4); lower Ricci bounds may fail and thus "Brownian motion may travel arbitrarily fast". Nevertheless, looking at the formula for the gradient $\nabla u(\cdot,T)_x$ and taking into account that

$$u(X_\tau(x), T-\tau) = \mathbb{E}^{\mathcal{F}_\tau}\left[1_{\{T<\zeta(x)\}}\, f(X_T(x))\right],$$

we see that Eq. (1.3) reads as

$$\langle \nabla u(\cdot,T)_x, v\rangle = -\mathbb{E}\left[1_{\{T<\zeta(x)\}}\, f(X_T(x)) \int_0^\tau \left\langle Q_s\, \dot{\ell}_s, dB_s\right\rangle\right]$$

where $\tau = \tau(x) \wedge T$ and $\tau(x)$ the first exit time of $X_\bullet(x)$ from an arbitrarily small chosen neighbourhood of x. In other words, as far as the gradient at (x,T) is concerned, Ricci curvature of M matters only locally about the point x.

No derivative of the heat equation appears in the right-hand side of Eq. (1.4), thus gradient formulas are well suitable for estimates, see [11]. Such inequalities easily allow to bound ∇u in terms of some uniform norm of u.

For positive solutions of the heat equation however one wants to do better: typically one seeks for pointwise estimates which allow (modulo additional terms if necessary) to control $\nabla u(\cdot,T)_x$ by $u(x,T)$.

Theorem 1.3 (Classical Li-Yau estimate [8]). *Let M be complete Riemannian manifold and assume that* $\mathrm{Ric} \geq -k$ *where* $k \geq 0$. *Let u be a strictly positive solution of*

$$\frac{\partial}{\partial t} u = \frac{1}{2} \Delta u \quad \text{on} \quad M \times \mathbb{R}_+$$

and let $a > 1$. *Then*

$$\left(\frac{|\nabla u|}{u} \right)^2 (x,T) - a \, \frac{\Delta u}{u}(x,T) \leq c(n,a) \left[k + \frac{1}{T} \right]. \tag{1.5}$$

If $\mathrm{Ric} \geq 0$, *i.e.* $k = 0$, *then the choice* $a = 1$ *is possible.*

It is a surprising fact which has been noticed by many people that no straightforward way to pass from Bismut type derivative formulas to Li-Yau type gradient estimates seems to exist.

Li-Yau type inequalities for positive solutions u of the heat equation aim at estimating $\nabla \log u$ rather than ∇u. This adds an interesting non-linearity to the problem which is better to deal with in terms of submartingales and Bismut type inequalities than in terms of martingales which are the underlying concept for Bismut formulas. This point of view has been worked out in [1] for local estimates in the elliptic case of positive harmonic functions. Such estimates in global form, i.e., for positive harmonic functions on Riemannian manifolds, are due to S.T. Yau [12]; local versions have been established by Cheng and Yau [6].

In this paper we pursue the approach via submartingales to study the parabolic case. Even if it is meanwhile quite standard to obtain Li-Yau type estimates in global form via analytic methods, local versions require often completely new arguments [5, 9, 10, 13].

In this paper we derive various submartingales which lead to the wanted estimates in a surprisingly simple way.

§2. Basic formulas related to positive solutions of the heat equation and some elementary submartingales

The following formulas for solutions of the heat equation on a Riemannian manifold depend on the fact that the solutions are strictly positive.

Lemma 2.1. *Let M be a Riemannian manifold (not necessarily complete) and let $u = u(x,t)$ be a positive solution of the heat equation*

$$\frac{\partial}{\partial t} u = \frac{1}{2} \Delta u \tag{2.1}$$

on $M \times [0,T]$. Then the following equalities hold:

$$\left(\frac{1}{2}\Delta - \partial_t\right)(\log u) = -\frac{1}{2}\frac{|\nabla u|^2}{u^2}, \tag{2.2}$$

$$\left(\frac{1}{2}\Delta - \partial_t\right)(u \log u) = \frac{1}{2}\frac{|\nabla u|^2}{u}, \tag{2.3}$$

$$\left(\frac{1}{2}\Delta - \partial_t\right)\frac{|\nabla u|^2}{u} = \frac{1}{u}\left|\operatorname{Hess} u - \frac{\nabla u \otimes \nabla u}{u}\right|^2 + \frac{\operatorname{Ric}(\nabla u, \nabla u)}{u}. \tag{2.4}$$

Proof. All three equalities are easily checked by direct calculation. Q.E.D.

Eq. (2.4) in Lemma 2.1 gives raise to some inequalities frequently used in the sequel and crucial for our approach. Most of our results are based on the following observation.

Corollary 2.2. *Let M be a Riemannian manifold of dimension n (not necessarily complete) and let $u = u(x,t)$ be a positive solution of the heat equation* (2.1)*. Then we have:*

$$\left(\frac{1}{2}\Delta - \partial_t\right)\frac{|\nabla u|^2}{u} \geq \frac{1}{nu}\left(\Delta u - \frac{|\nabla u|^2}{u}\right)^2 + \frac{\operatorname{Ric}(\nabla u, \nabla u)}{u}. \tag{2.5}$$

If $\operatorname{Ric} \geq -k$ *on M for some $k \geq 0$, then*

$$\left(\frac{1}{2}\Delta - \partial_t\right)\frac{|\nabla u|^2}{u} \geq \frac{1}{nu}\left(\Delta u - \frac{|\nabla u|^2}{u}\right)^2 - k\,\frac{|\nabla u|^2}{u}, \tag{2.6}$$

and in particular,

$$\left(\frac{1}{2}\Delta - \partial_t\right)\frac{|\nabla u|^2}{u} \geq -k\,\frac{|\nabla u|^2}{u}. \tag{2.7}$$

Proof. This is a direct consequence of Eq. (2.4). Q.E.D.

Lemma 2.3. *Let M be a Riemannian manifold (not necessarily complete) and let $u(x,t) = P_t f(x)$ be a positive solution of the heat equation*

$$\frac{\partial}{\partial t}u = \frac{1}{2}\,\Delta u \tag{2.8}$$

on $M \times [0,T]$. For any Brownian motion X on M, the process

$$m_t^1 := \frac{|\nabla P_{T-t} f|^2}{P_{T-t} f}(X_t)\, \exp\left\{-\int_0^t \underline{\operatorname{Ric}}(X_r)\, dr\right\}, \tag{2.9}$$

where $\underline{\mathrm{Ric}}(x)$ *denotes the smallest eigenvalue of the Ricci curvature at the point* x*, is a local submartingale (up to its natural lifetime). Furthermore*

$$m_t^2 := \big(\log P_{T-t}f\big)(X_t) + \frac{1}{2}\int_0^t \left|\frac{\nabla P_{T-s}f}{P_{T-s}f}\right|^2 (X_s)\,ds \tag{2.10}$$

$$m_t^3 := \big(P_{T-t}f \log P_{T-t}f\big)(X_t) - \frac{1}{2}\int_0^t \frac{|\nabla P_{T-s}f|^2}{P_{T-s}f}(X_s)\,ds \tag{2.11}$$

are local martingales (up to their respective lifetimes).

Proof. The first claim is a consequence of (2.5); the second part comes from Eqs. (2.2) and (2.3). Q.E.D.

Lemma 2.4. *Let* M *be a Riemannian manifold and* $u(x,t) = P_t f(x)$ *be a positive solution of the heat equation* (2.8) *on* $M \times [0,T]$*. If* $\mathrm{Ric} \geq -k$ *for some* $k \geq 0$*, then for any Brownian motion* X *on* M*, the process*

$$N_t := \frac{T-t}{2(1+k(T-t))}\,\frac{|\nabla P_{T-t}f|^2}{P_{T-t}f}(X_t) + \big(P_{T-t}f \log P_{T-t}f\big)(X_t) \tag{2.12}$$

is a local submartingale (up to its lifetime).

Proof. The proof follows from Itô's formula using inequality (2.7), along with Eq. (2.3). Q.E.D.

§3. Global gradient estimates

In this section we explain how submartingales related to positive solutions of the heat equation can be turned into gradient estimates. The resulting estimates of this section are classical inequalities; our focus lies on the stochastic approach.

The main problem in the subsequent sections will then be to use methods of Stochastic Analysis to derive localized versions of the bounds. The following gradient estimates follow immediately from Lemma 2.4.

Theorem 3.1 (Entropy estimate)**.** *Let* $u(x,t) = P_t f(x)$ *be a positive solution of the heat equation on a compact manifold* M*. Assume that* $\mathrm{Ric} \geq -k$ *for some* $k \geq 0$*. Then*

$$\left|\frac{\nabla P_T f}{P_T f}\right|^2 (x) \leq 2\left(\frac{1}{T} + k\right) P_T\left(\frac{f}{P_T f(x)} \log \frac{f}{P_T f(x)}\right)(x). \tag{3.1}$$

Proof. Indeed if M is compact, then the local submartingale N_t in (2.12) is a true submartingale. Let

$$h(t) = \frac{T-t}{2(1+k(T-t))}.$$

Then, evaluating $\mathbb{E}[N_0] \leq \mathbb{E}[N_T]$, we obtain

$$h(0)\,\frac{|\nabla P_T f|^2}{P_T f}(x) + P_T f(x) \log P_T f(x) \leq P_T(f \log f)(x),$$

or in other words,

$$\frac{|\nabla P_T f|^2}{P_T f}(x) \leq \frac{1}{h(0)}\, P_T\left(f \log \frac{f}{P_T f(x)}\right)(x).$$

Dividing through $P_T f(x)$ completes the proof. Q.E.D.

Corollary 3.2. *Keeping notation and assumptions of Theorem* 3.1 *we observe that, for any* $\delta > 0$,

$$\begin{aligned} |\nabla P_T f(x)| \leq\ & \frac{1}{2\delta}\left(\frac{1}{T} + k\right) P_T f(x) \\ & + \delta\left[P_T\left(f \log f\right)(x) - P_T f(x) \log P_T f(x)\right]. \end{aligned} \tag{3.2}$$

Proof. Indeed with $h(0) = T/(2 + 2kT)$, we conclude from (3.1) that

$$\begin{aligned} \frac{|\nabla P_T f|}{P_T f}(x) &\leq \sqrt{\frac{1}{2\delta\, h(0)}}\, \sqrt{2\delta\, P_T\left(\frac{f}{P_T f(x)} \log \frac{f}{P_T f(x)}\right)(x)} \\ &\leq \frac{1}{2\delta}\left(\frac{1}{T} + k\right) + \delta\, P_T\left(\frac{f}{P_T f(x)} \log \frac{f}{P_T f(x)}\right)(x). \end{aligned}$$

Q.E.D.

Corollary 3.3 (Hamilton [7])**.** *Let* M *be a compact Riemannian manifold such that* $\mathrm{Ric} \geq -k$ *throughout* M *for some* $k \geq 0$. *Suppose that* $u(x,t)$ *is a positive solution of the heat equation* (2.8) *on* $M \times [0,T]$, *and let* $A := \sup_{M\times[0,T]} u$. *Then*

$$\frac{|\nabla u|^2}{u^2}(x,T) \leq 2\left(\frac{1}{T} + k\right) \log \frac{A}{u(x,T)}\,. \tag{3.3}$$

In particular, if $\mathrm{Ric} \geq 0$ *then*

$$\frac{|\nabla u|}{u}(x,T) \leq \frac{1}{T^{1/2}} \sqrt{2 \log \frac{A}{u(x,T)}}\,. \tag{3.4}$$

Proof. The proof of (3.3) is an application of Theorem 3.1, along with the observation that $P_T f^*(x) = 1$ when f is normalized as $f^* := f/P_T f(x)$ for fixed x. Q.E.D.

Remark 3.4. In the proofs above compactness of the manifold has only been used to assure that the local submartingale (2.12) is a true submartingale. The results extend to bounded positive solution of the heat equation on complete manifolds with lower Ricci bounds. Indeed, $u(x,t) = P_t f(x)$ may be assumed to be bounded away from 0 (otherwise one may first pass to $u^* := u + \varepsilon$ and let $\varepsilon > 0$ tend to 0 in the obtained estimate). The term $(T-t)\,|\nabla P_{T-t} f|^2$ may be bounded by Bismut's formula, see [11].

We now turn to the classical Li-Yau estimate (1.5). Let M be a given complete Riemannian manifold of dimension n such that $\mathrm{Ric} \geq -k$ for some $k \geq 0$. Suppose that u is a positive solution to the heat equation (2.8) on $M \times [0,T]$. Starting from (2.6) in Corollary 2.2 we have

$$\left(\frac{1}{2}\Delta - \partial_t\right) \frac{|\nabla u|^2}{u} \geq \frac{1}{nu}\left(\Delta u - \frac{|\nabla u|^2}{u}\right)^2 - k\frac{|\nabla u|^2}{u}, \tag{3.5}$$

and thus

$$\left(\frac{1}{2}\Delta - \partial_t\right) \frac{|\nabla u|^2}{u} \geq \frac{1}{nu}\, q^2 - k\, q - k\, \Delta u, \tag{3.6}$$

where

$$q := \frac{|\nabla u|^2}{u} - \Delta u = \frac{|\nabla u|^2}{u} - 2\,\partial_t u.$$

Fixing $x \in M$, let $X = X(x)$ be a Brownian motion on M starting at x. Our first goal is to investigate the process

$$\left(h_t\, \frac{|\nabla u|^2}{u}(X_t, T-t)\right)_{t \geq 0}$$

where $h_t = \ell_t^2$ for some adapted continuous real-valued process ℓ_t with absolutely continuous paths such that $\ell_0 = 1$ and $\ell_T = 0$.

Let $q_t = q(X_t, T-t)$, $u_t = u(X_t, T-t)$ and $(\Delta u)_t = \Delta u(X_t, T-t)$. Using (3.6) we find (modulo differentials of local martingales)

$$d\left(h_t\, \frac{|\nabla u|^2}{u}(X_t, T-t)\right) \tag{3.7}$$

$$\geq \left[\dot{h}_t q_t + \frac{h_t}{nu_t}\, q_t^2 - k\, q_t h_t + \left(\dot{h}_t - k\, h_t\right)(\Delta u)_t\right] dt. \tag{3.8}$$

Minimizing the term

$$\frac{h_t}{nu_t}\, q_t^2 + (\dot{h}_t - k\, h_t) q_t$$

as a quadratic function of q_t, we find

$$\frac{h_t}{nu_t}\, q_t^2 + (\dot{h}_t - k\, h_t) q_t \geq -\frac{(\dot{h}_t - k\, h_t)^2}{4h_t}\, nu_t.$$

Thus, integrating (3.7) from 0 to T and taking expectations, we obtain

(3.9)
$$\frac{|\nabla u|^2}{u}(x,T) \leq \mathbb{E}\left[\int_0^T \left(n\, \frac{(\dot{h}_t - k\, h_t)^2}{4h_t}\, u_t + (kh_t - \dot{h}_t)(\Delta u)_t\right) dt\right]$$

Theorem 3.5 (Li-Yau inequality for $\mathrm{Ric} \geq 0$)**.** *Let M be a complete Riemannian manifold of dimension n such that* $\mathrm{Ric} \geq 0$*. Let $u = u(x,t)$ be a positive bounded solution of the heat equation* (2.8) *on $M \times [0,T]$. Then, for each $x \in D$,*

$$\frac{|\nabla u|^2}{u^2}(x,T) - \frac{\Delta u}{u}(x,T) \leq n\, \mathbb{E}\left[\int_0^T |\dot{\ell}_t|^2\, \frac{u(X_t(x), T-t)}{u(x,T)}\, dt\right] \tag{3.10}$$

where (ℓ_t) is an adapted continuous real-valued process ℓ_t with absolutely continuous paths such that $\ell_0 = 1$ and $\ell_T = 0$.

In particular, with the choice $\ell_t := (T-t)/T$, we obtain

$$\frac{|\nabla u|^2}{u^2}(x,T) - \frac{\Delta u}{u}(x,T) \leq \frac{n}{T}\,.$$

which is the classical estimate of Li-Yau.

Proof. By (3.7) we have

$$\frac{|\nabla u|^2}{u}(x,T) \leq \mathbb{E}\left[\int_0^T \left(n\, \frac{|\dot{h}_t|^2}{4h_t}\, u_t - \dot{h}_t\, (\Delta u)_t\right) dt.\right] \tag{3.11}$$

First note that Δu is a solution of the heat equation as well, hence $(\Delta u)_t$ a local martingale. In particular,

$$d\big(h_t\, (\Delta u)_t\big) \stackrel{\mathrm{m}}{=} \dot{h}_t\, (\Delta u)_t\, dt,$$

where $\stackrel{\mathrm{m}}{=}$ stands for equality modulo differentials of local martingales, and hence

$$\mathbb{E}\left[\int_0^T \dot{h}_t\, (\Delta u)_t\, dt\right] = -h_0\, (\Delta u)_0 = -\Delta u(x,T).$$

Thus (3.11) shows that

$$\frac{|\nabla u|^2}{u^2}(x,T) - \frac{\Delta u}{u}(x,T) \le n\,\mathbb{E}\left[\int_0^T \dot{\ell}_t^2\,\frac{u_t}{u_0}\,dt\right] = n\,\mathbb{E}\left[\int_0^T \dot{\ell}_t^2\,dt\cdot\frac{u_T}{u_0}\right].$$

Q.E.D.

Remarks 3.6. (i) Using (3.9), Theorem 3.5 is easily extended to the case of a lower Ricci bound. For local versions of the Li-Yau's estimate one could try to modify the process ℓ_t in such a way that ℓ_t already vanishes as soon as the Brownian motion X_t reaches the boundary of D. We shall not pursue this approach here, but rather adopt an even simpler argument in the next section which leads to the local estimate.

(ii) Of particular interest are localized versions of the entropy estimates (3.1) and (3.2). Such estimates lead to Harnack inequalities and heat kernel bounds, valid on arbitrary manifolds without bounded geometry, see [2, 3]. Results in this direction will be worked out elsewhere [4].

§4. Local Li-Yau type inequalities

Our main task of the remaining sections will be to localize the arguments of Section 3 to cover local solutions of the heat equation on bounded domains. We start with the Li-Yau estimate.

Assumption 1. Let M be a complete Riemannian manifold of dimension n, and let $u = u(x,t)$ be a solution of the heat equation (2.8) on $D\times[0,T]$ where $D \subset M$ is a relatively compact open subset of M with nonempty smooth boundary. Assume that u is positive and continuous on $\bar{D} \times [0,T]$. Furthermore let

$$k := \inf\big\{\mathrm{Ric}_x(v,v) : v \in T_xM,\ |v| = 1,\ x \in D\big\} \tag{4.1}$$

be a lower bound for the Ricci curvature on the domain D. Finally let $\varphi \in C^2(\bar{D})$ with $\varphi > 0$ in D and $\varphi|\partial D = 0$.

Assumption 2. Let $x \in D$ and $X(x)$ be a Brownian motion on M starting at x at time 0. Denote by $\tau(x)$ its first exit time of D.

Now, for $t \in [0, T \wedge \tau(x)[$, consider the process

$$Y_t = C_1\,(T-t)^{-1} + C_2\,\varphi^{-2}(X_t(x)) + \alpha k, \tag{4.2}$$

where C_1, $C_2 > 0$ are constants which will be specified later.

Let h_t be the solution of

$$\dot{h}_t = -h_t Y_t, \qquad h_0 = 1; \tag{4.3}$$

in other words,

$$h_t = \exp\left\{ -\int_0^t \left(\frac{C_1}{T-r} + \frac{C_2}{\varphi^2(X_r(x))} + \alpha k \right) dt \right\}.$$

Then, letting

$$q_t = \left(\frac{|\nabla u|^2}{u} - \Delta u \right)(X_t, T-t),$$

we find (modulo differentials of local martingales)

$$d(h_t q_t) \geq \left[h_t \frac{q_t^2}{n u_t} + \left(\dot{h}_t - k h_t \right) q_t - k h_t (\Delta u)_t \right] dt. \tag{4.4}$$

Thus letting

$$S_t := h_t q_t + n u_t \dot{h}_t \equiv h_t \left(q_t - n u_t Y_t \right), \quad t \in [0, T \wedge \tau(x)[, \tag{4.5}$$

we get (modulo differentials of local martingales)

$$\begin{aligned} dS_t &= d(h_t q_t) - n u_t \, d(h_t Y_t) + n \, d[u, \dot{h}]_t \\ &\geq \left[h_t \frac{q_t^2}{n u_t} + \left(\dot{h}_t - k h_t \right) q_t - k h_t (\Delta u)_t \right] dt \\ &\quad + n u_t \, h_t Y_t^2 \, dt \\ &\quad - n u_t h_t \left[C_1 \, (T-t)^{-2} + C_2 \, c_\varphi(X_t) \, \varphi^{-4}(X_t) \right] dt \\ &\quad - n C_2 \, h_t \, d[u, \varphi^{-2}(X(x))]_t \end{aligned}$$

where the bracket $[\cdot, \cdot]$ stands for quadratic covariation on the space of continuous semimartingales and where

$$c_\varphi(x) = \left(3|\nabla \varphi|^2 - \varphi \Delta \varphi \right)(x). \tag{4.6}$$

On the other hand, denoting again

$$\begin{aligned} u_t &= u(T-t, \cdot)(X_t), \\ \nabla u_t &= \nabla u(T-t, \cdot)(X_t) \end{aligned} \tag{4.7}$$

and

$$\Delta u_t = \Delta u(T-t, \cdot)(X_t), \tag{4.8}$$

we have for any $\alpha > 0$,

$$\begin{aligned}
&-nC_2\, h_t\, d[u, \varphi^{-2}(X_t)]_t \\
&\quad = nC_2\, h_t 2\varphi^{-3}(X_t)\langle \nabla u_t, \nabla\varphi(X_t)\rangle\, dt \\
&\quad \geq -2nC_2\, h_t \varphi^{-3}(X_t)|\nabla u_t|\, |\nabla\varphi(X_t)|\, dt \\
&\quad = -2nC_2\, h_t \left(\varphi^{-1}(X_t)\, (\alpha n u_t)^{-1/2}\, |\nabla u_t|\right) \\
&\qquad \times \left((\alpha n u_t)^{1/2} (\varphi^{-2}|\nabla\varphi|)(X_t)\right)\, dt \\
&\quad \geq \left(-\alpha^{-1} C_2\, h_t \varphi^{-2}(X_t)(q_t + \Delta u_t) - C_2\, \alpha n^2 u_t h_t \varphi^{-4} |\nabla\varphi|^2(X_t)\right)\, dt \\
&\quad \geq \left(-\alpha^{-1} h_t (Y_t - \alpha k)(q_t + \Delta u_t) - C_2\, \alpha n^2 u_t h_t \varphi^{-4} |\nabla\varphi|^2(X_t)\right)\, dt \\
&\quad = \left(\left(\alpha^{-1}\dot{h}_t + k h_t\right)(q_t + \Delta u_t) - C_2\, \alpha n^2 u_t h_t \varphi^{-4} |\nabla\varphi|^2(X_t)\right)\, dt.
\end{aligned}$$

Hence letting, for $\alpha > 0$,

$$S_{\alpha,t} = h_t \left(q_t - \alpha^{-1}\Delta u_t\right) + n u_t \dot{h}_t \tag{4.9}$$

we get

$$\begin{aligned}
dS_{\alpha,t} \geq &\left[h_t \frac{q_t^2}{n u_t} + \left(1 + \alpha^{-1}\right) \dot{h}_t\, q_t\right] dt \\
&+ h_t Y_t^2\, n u_t\, dt \\
&- n u_t h_t \Big[C_1 (T-t)^{-2} + C_2\, C_{\varphi,\alpha,n}\, \varphi^{-4}(X_t)\Big]\, dt
\end{aligned}$$

where

$$C_{\varphi,\alpha,n} = \sup_D \left\{c_\varphi + \alpha n |\nabla\varphi|^2\right\} = \sup_D \left\{(3 + \alpha n)|\nabla\varphi|^2 - \varphi\Delta\varphi\right\}. \tag{4.10}$$

Minimizing the first line on the right hand side, we find

$$\begin{aligned}
dS_{\alpha,t} \geq\, & h_t\, Y_t^2\, n u_t \left(\frac{4 - (1 + \alpha^{-1})^2}{4}\right)\, dt \\
& - n u_t\, h_t \Big[C_1\, (T-t)^{-2} + C_2\, C_{\varphi,\alpha,n}\, \varphi^{-4}(X_t)\Big]\, dt.
\end{aligned}$$

Putting things together, we arrive at the following result.

Lemma 4.1. *We keep notation and assumptions from above. Assume that $\alpha > 1$ and let*

$$C_1 \geq C_1(\alpha) := \frac{4}{4 - (1 + \alpha^{-1})^2} \tag{4.11}$$

and

$$C_2 \geq C_2(\varphi,\alpha,n) := \frac{4}{4-(1+\alpha^{-1})^2}\,\sup_D\Big\{(3+\alpha n)|\nabla\varphi|^2-\varphi\Delta\varphi\Big\}. \tag{4.12}$$

Then $S_{\alpha,t}$ is a local submartingale on $[0,T\wedge\tau(x)[$.

Proof. Using

$$Y_t^2 \geq C_1^2\,(T-t)^{-2}+C_2^2\,\varphi^{-4}(X_t), \tag{4.13}$$

we get

$$\begin{aligned} dS_{\alpha,t} \geq\ & h_t n u_t\, C_1\left(\frac{4-(1+\alpha^{-1})^2}{4}\,C_1-1\right)(T-t)^{-2}\,dt \\ & + h_t n u_t\, C_2\left(\frac{4-(1+\alpha^{-1})^2}{4}\,C_2-C_{\varphi,\alpha,n}\right)\varphi^{-4}(X_t)\,dt. \end{aligned}$$

Thus, under condition (4.11) and (4.12), the right-hand side is nonnegative. Q.E.D.

Theorem 4.2 (Li-Yau inequality; local version)**.** *We keep the assumptions from above. Let $u=u(x,t)$ be a solution of the heat equation on $D\times[0,T]$ which is positive and continuous on $\bar{D}\times[0,T]$.*

For any $\alpha\in\,]1,\infty[$, we have

$$\frac{|\nabla u_0|^2}{u_0^2}-(1+\alpha^{-1})\,\frac{\Delta u_0}{u_0} \leq \frac{n\,C_1(\alpha)}{T}+\frac{n\,C_2(\varphi,\alpha,n)}{\varphi^2(x)}+n\alpha k, \tag{4.14}$$

where k is a lower Ricci bound on the domain D, and where $C_1(\alpha)$ and $C_2(\varphi,\alpha,n)$ are specified in (4.11)*, resp.* (4.12)*. The function φ is as in Assumption* 1*.*

Recall that $u_0=u(\cdot,T)$ and $\Delta u_0=\Delta u(\cdot,T)$ according to (4.7)*, resp.* (4.8)

Proof. Let

$$C_1=C_1(\alpha) \quad\text{and}\quad C_2=C_2(\varphi,\alpha,n).$$

Consider

$$S_{\alpha,t}=h_t\left(q_t-\alpha^{-1}\Delta u_t-nu_tY_t\right).$$

We assume that $S_{\alpha,0}>0$ and let τ_α be the first hitting time of 0 by $S_{\alpha,t}$. Then clearly $\tau_\alpha<T\wedge\tau(x)$, since

$$q_t-\alpha^{-1}\Delta u_t-nu_tY_t$$

converges to $-\infty$ as t tends to $T \wedge \tau(x)$.

Let

$$K := \max_{\bar{D}\times[0,T]} (q - \alpha^{-1}\Delta u) \quad \text{and} \quad m = \min_{\bar{D}\times[0,T]} u.$$

Then, for $t \in [0, \tau_\alpha]$, we have $S_t \geq 0$, which implies $Y_t \leq K/nm$. From this we easily prove that on $[0, \tau_\alpha]$, the process $S_{\alpha,t}$ is a submartingale with bounded local characteristics. As a consequence, we have

$$S_{\alpha,0} \leq \mathbb{E}[S_{\alpha,\tau_\alpha}].$$

Since $S_{\alpha,\tau_\alpha} \equiv 0$, this contradicts the assumption $S_{\alpha,0} > 0$. Hence we must have $S_{\alpha,0} \leq 0$, which is the desired inequality. Q.E.D.

Remark 4.3. In the case of a global solution of the heat equation on a compact manifold, we can take φ as a constant and then $C_2(\alpha, \varphi, n) = 0$. If moreover $k = 0$, then one can take $C_2 = 0$ and $C_1 = 1$, and S_t is a local submartingale. This recovers one more time the usual Li-Yau estimate

$$\frac{|\nabla u_0|^2}{u_0^2} - \frac{\Delta u_0}{u_0} \leq \frac{n}{T}\,. \tag{4.15}$$

A similar reasoning applies for global solutions on complete Riemannian manifolds with a lower Ricci curvature bound.

§5. Li-Yau inequality with lower order term

We keep Assumption 1 and 2 of Section 4 as standing assumptions for the rest of the paper and study now the process

$$S_t' = q_t - nu_t Z_t \tag{5.1}$$

where

$$Z_t = C_1\,(T-t)^{-1} + C_2\,\varphi^{-2}(X_t) + C_3$$

with constants $C_1, C_2, C_3 > 0$ to be specified later.

Let

$$C_\varphi = \sup_D \left\{3|\nabla\varphi|^2 - \varphi\Delta\varphi\right\}. \tag{5.2}$$

Then we have

$$\begin{aligned} dS'_t \geq & \left[\frac{q_t^2}{nu_t} - k\frac{|\nabla u_t|^2}{u_t} - nu_t \left(C_1 (T-t)^{-2} + C_2\, C_\varphi\, \varphi^{-4}(X_t) \right) \right] dt \\ & - C_2\, nd\, [\varphi^{-2}(X), u]_t \\ \geq & \left[\frac{q_t^2}{nu_t} - nu_t \left(\frac{C_1}{(T-t)^2} + \frac{C_2\, C_\varphi}{\varphi^4(X_t)} + \frac{k}{n} \left\| \frac{|\nabla u|}{u} \right\|^2_{\bar{D}\times[0,T]} \right) \right] dt \\ & - 2C_2\, nu_t \left\| \frac{|\nabla u|}{u} \right\|_{\bar{D}\times[0,T]} \|\varphi \nabla \varphi\|^2_D\, \varphi^{-4}(X_t)\, dt \\ \geq & \left[\frac{q_t^2}{nu_t} - nu_t \left(\frac{C_1}{(T-t)^2} + \frac{C_2}{\varphi^4(X_t)} \right.\right. \\ & \left.\left. \times \left(C_\varphi + 2 \left\| \frac{|\nabla u|}{u} \right\|_{\bar{D}\times[0,T]} \|\varphi \nabla \varphi\|_D \right) \right) \right] dt \\ & - nu_t\, \frac{k}{n} \left\| \frac{|\nabla u|}{u} \right\|^2_{\bar{D}\times[0,T]} dt. \end{aligned}$$

Lemma 5.1. *Let*

$$\begin{aligned} & C_1 = 1, \quad C_2 = C_\varphi + 2 \left\| \frac{|\nabla u|}{u} \right\|_{\bar{D}\times[0,T]} \|\varphi \nabla \varphi\|_\infty \quad \textit{and} \\ & C_3 = \sqrt{\frac{k}{n}} \left\| \frac{|\nabla u|}{u} \right\|_{\bar{D}\times[0,T]}. \end{aligned} \tag{5.3}$$

Then on $\{S'_t \geq 0\}$, *the process* S'_t *has nonnegative drift.*

Proof. We have

$$Z_t^2 \geq C_1^2 (T-t)^{-2} + C_2^2 \varphi^{-4}(X_t) + C_3^2.$$

Consequently, under condition (5.3),

$$dS'_t \geq \frac{1}{nu_t} \left(q_t^2 - (nu_t Z_t)^2 \right) dt = \frac{S'_t}{nu_t} \left(q_t + nu_t Z_t \right) dt$$

and the right-hand side is nonnegative on $\{S'_t \geq 0\}$. Q.E.D.

Similarly to Theorem 4.2, we obtain the following result.

Theorem 5.2 (Local Li-Yau inequality with lower order term)**.** *We keep the notation from above, as well as Assumption* 1 *and* 2 *from Section* 4*. Let $u = u(x,t)$ be a solution of the heat equation on $D \times [0,T]$ which is positive and continuous on $\bar{D} \times [0,T]$. Then*

$$\frac{|\nabla u_0|^2}{u_0^2} - \frac{\Delta u_0}{u_0} \leq \frac{n}{T} + \frac{nC_\varphi}{\varphi^2(x)} + \left(\sqrt{nk} + \frac{2n\,\|\varphi \nabla \varphi\|_D}{\varphi^2(x)}\right) \left\| \frac{|\nabla u|}{u} \right\|_{\bar{D}\times[0,T]}.$$

§6. Local gradient estimates of Hamilton type

We keep Assumptions 1 and 2 of Section 4 and study now the process

$$S_t = \frac{|\nabla u_t|}{2u_t} - u_t(1 - \log u_t)^2 Z_t, \tag{6.1}$$

where

$$Z_t = \frac{C_1}{(T-t)} + \frac{C_2}{\varphi^2(X_t)} + C_3$$

for some constants C_1, C_2, $C_3 > 0$.

Assume that $0 < u \leq e^{-3}$ (this assumption will be removed in Theorem 6.1 through replacing u by $e^{-3}\, u/\|u\|_{\bar{D}\times[0,T]}$). Let $c_\varphi(x)$ again be given by (4.6). Then, denoting

$$g(t,x) = \frac{|\nabla u|^2}{u}(t,x) \quad \text{and} \quad g_t = g(T-t, X_t),$$

and using the fact that

$$\nabla \left(u(1-\log u)^2\right) = (\log^2 u - 1)\nabla u$$

and

$$d\left(u_t(1-\log u_t)^2\right) \stackrel{\mathrm{m}}{=} g_t \log u_t \, dt,$$

we get

$$\begin{aligned} dS_t \geq & -k\,\frac{1}{2}\, g_t\, dt \\ & - u_t(1-\log u_t)^2 \Big(C_1\,(T-t)^2 + C_2\, c_\varphi(X_t)\varphi^{-4}(X_t) \Big)\, dt \\ & - 2\log u_t\, \frac{1}{2}\, g_t Z_t\, dt \\ & - 2C_2(1-\log u_t)(1+\log u_t)\varphi^{-3}(X_t)\, \langle \nabla u_t, \nabla \varphi(X_t)\rangle\, dt. \end{aligned}$$

Now from $u \le e^{-3}$ we get

$$-2\log u_t \ge 3(1-\log u_t)/2.$$

This together with $|1+\log u_t| \le 1-\log u_t$ yields (modulo differentials of local martingales)

$$\begin{aligned}
dS_t &\ge (1-\log u_t)\Bigg\{ \left[\left(\frac{3}{2}Z_t - k\right)\frac{1}{2}\, g_t \right. \\
&\quad \left. - u_t(1-\log u_t)\left(C_1(T-t)^2 + C_2 c_\varphi(X_t)\varphi^{-4}(X_t)\right)\right] dt \\
&\quad - C_2\left[(1-\log u_t)\, 2\sqrt{2}\,\varphi^{-2}(X_t)\,|\nabla\varphi(X_t)|\,\sqrt{u_t}\,\varphi^{-1}(X_t)\,\sqrt{\frac{g_t}{2}}\,\right] dt\Bigg\} \\
&\ge (1-\log u_t)\Bigg\{ \left[\left(\frac{3}{2}Z_t - k\right)\frac{1}{2}\, g_t \right. \\
&\quad \left. - u_t(1-\log u_t)\left(C_1(T-t)^2 + C_2 c_\varphi(X_t)\varphi^{-4}(X_t)\right)\right] dt \\
&\quad - \left[(1-\log u_t)^2 u_t\, 4C_2\varphi^{-4}(X_t)\,|\nabla\varphi(X_t)|^2 + \frac{1}{4}g_t C_2\varphi^{-2}(X_t)\right] dt\Bigg\} \\
&\ge (1-\log u_t)\Bigg[(Z_t-k)\,\frac{1}{2}\, g_t - u_t(1-\log u_t)^2 \\
&\quad \times \left(C_1(T-t)^2 + C_2\left(c_\varphi(X_t) + 4|\nabla\varphi(X_t)|^2\right)\varphi^{-4}(X_t)\right)\Bigg] dt.
\end{aligned}$$

Letting

$$C_1 = 1, \quad C_2 = \sup_D \left\{c_\varphi + 4|\nabla\varphi|^2\right\} \quad \text{and} \quad C_3 = k, \tag{6.2}$$

we get

$$\begin{aligned}
dS_t &\ge (1-\log u_t)\left[(Z_t-k)\frac{1}{2}\, g_t - u_t(1-\log u_t)^2(Z_t-k)^2\right] dt \\
&\ge (1-\log u_t)(Z_t-k)\left[\frac{1}{2}\, g_t - u_t(1-\log u_t)^2 Z_t\right] dt.
\end{aligned}$$

This proves that S_t has nonnegative drift on $\{S_t \ge 0\}$. On the other hand, S_t converges to $-\infty$ as $t \to T \wedge \tau(x)$.

Similarly to Theorem 4.2, we obtain the following result.

Theorem 6.1 (Local Li-Yau inequality of Hamilton type)**.** *We keep the assumptions as above. Assume that u is a solution of the heat equation on $D \times [0,T]$ which is positive and continuous on $\bar{D} \times [0,T]$. Then*

$$\left|\frac{\nabla u_0}{u_0}\right|^2 \leq 2\left(\frac{1}{T} + \frac{\sup_D \left\{7|\nabla\varphi|^2 - \varphi\Delta\varphi\right\}}{\varphi^2(x)} + k\right)\left(4 + \log\frac{\|u\|_{\bar{D}\times[0,T]}}{u_0}\right)^2$$

where φ is as above.

§7. Explicit upper bounds

The estimates in Theorems 4.2, 5.2 and 6.1 have been given in terms of a function $\varphi \in C^2(\bar{D})$ such that $\varphi > 0$ in D and $\varphi|\partial D = 0$. To specify the constants an explicit choice for φ has to be done.

We fix $x \in D$ and let $\delta_x = \rho(x, \partial D)$ where ρ denotes the Riemannian distance. We replace D by the ball $B = B(x, \delta_x)$ and consider on B

$$\varphi(y) = \cos\frac{\pi\rho(x,y)}{2\delta_x}. \tag{7.1}$$

Clearly $\varphi(x) = 1$, φ is nonnegative and bounded by 1, and φ vanishes on ∂B.

It is proven in [11] that

$$d\varphi^{-2}(X_t) \leq \frac{1}{2}\Delta(\varphi^{-2})(X_t)\,dt \tag{7.2}$$

where by convention $\Delta\varphi^{-2} = 0$ at points where φ^{-2} is not differentiable. Moreover, since the time spent by X_t on the cut-locus of x is a.s. zero, the differential of the brackets $[\varphi(X_t), u_t]$ may be taken as 0 at points where φ^{-2} is not differentiable. As a consequence, all estimates in Theorems 4.2, 5.2 and 6.1 remain valid with φ defined by (7.1).

We are now going to derive explicit expressions for the constants. To this end we observe that

$$\|\nabla\varphi\|_B \leq \frac{\pi}{2\delta_x}.$$

From [11], we get

$$-\Delta\varphi \leq \frac{\pi\sqrt{k(n-1)}}{2\delta_x} + \frac{\pi^2 n}{4\delta_x^2}$$

which gives for any $\beta > 0$,

$$-\Delta\varphi \leq \frac{\pi^2(1+\beta)n}{4\delta_x^2} + \frac{k}{4\beta}.$$

This yields

$$C_\varphi \le \frac{\pi^2\left[(1+\beta)n+3\right]}{4\delta_x^2} + \frac{k}{4\beta},$$

$$C_{\varphi,\alpha,n} \le \frac{\pi^2\left[(1+\beta+\alpha)n+3\right]}{4\delta_x^2} + \frac{k}{4\beta},$$

$$\sup_D \left\{7|\nabla\varphi|^2 - \varphi\Delta\varphi\right\} \le \frac{\pi^2\left[(1+\beta)n+7\right]}{4\delta_x^2} + \frac{k}{4\beta}.$$

Finally we replace α by $a = 1+\alpha^{-1}$ to obtain from Theorems 4.2, 5.2 and 6.1 the following explicit upper bounds.

Theorem 7.1 (Local Li-Yau inequalities with explicit constants)**.** *Let u be a solution of the heat equation on $D\times[0,T]$ where D is a relatively compact open subset of a Riemannian manifold M. Assume that u is positive and continuous on $\bar{D}\times[0,T]$. Furthermore let k be a lower bound for the Ricci curvature on the domain D.*

Fix $x\in D$ and let $a\in\,]1,2[$. For any $\beta>0$ we have

$$\begin{aligned}\left|\frac{\nabla u_0}{u_0}\right|^2 - a\frac{\Delta u_0}{u_0} &\le \frac{4n}{(4-a^2)T} + \frac{\pi^2 n\left[\left(1+\beta+\frac{1}{a-1}\right)n+3\right]}{(4-a^2)\delta_x^2} \\ &\quad + \left(\frac{1}{(4-a^2)\beta}+\frac{1}{a-1}\right)nk,\\ \left|\frac{\nabla u_0}{u_0}\right|^2 - \frac{\Delta u_0}{u_0} &\le \frac{n}{T} + \frac{n\pi^2\left[(1+\beta)n+3\right]}{4\delta_x^2} + \frac{nk}{4\beta}\\ &\quad + \sqrt{nk}\left\|\frac{|\nabla u|}{u}\right\|_{\bar{D}\times[0,T]} + \frac{n\pi}{\delta_x}\left\|\frac{|\nabla u|}{u}\right\|_{\bar{D}\times[0,T]}\end{aligned}$$

and

$$\begin{aligned}\left|\frac{\nabla u_0}{u_0}\right|^2 &\le 2\left(\frac{1}{T} + \frac{\pi^2\left[(1+\beta)n+7\right]}{4\delta_x^2} + \left(\frac{1}{4\beta}+1\right)k\right)\\ &\quad\times\left(4+\log\frac{\|u\|_{\bar{D}\times[0,T]}}{u_0}\right)^2\end{aligned}$$

where n denotes the dimension of M and δ_x the Riemannian distance of x to the boundary of D. Recall that $u_0 = u(\cdot,T)$ and $\Delta u_0 = \Delta u(\cdot,T)$.

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