New Heat Kernel Estimates on Riemannian Manifolds with Negative Curvature
(Partial work join with Junfang Li, UAB)

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Outline

• Problem setting

• Some History

• Li-Yau type Differential Harnack inequality

• Upper bound estimates for Heat kernel $H(x, y, t)$

• Lower bounds estimates for Heat kernel $H(x, y, t)$

• References
**Problem setting**

- \((M^n, g)\): a complete Riemannian manifold with \(\text{Ricci}(M) \geq -k\),

**Heat Equation:**

\[
u_t = \Delta_g u, \quad u(x, 0) = u_0(x) \quad \text{on } M;
\]

**Solution:**

\[
u(x, t) = e^{-t\Delta_g} u_0(x) = \int_M H(x, y, t) u_0(y) dy
\]

where \(H(x, y, t)\): the heat kernel (the fundamental solution) of \(M\).

**Gaussian Kernel:**

\[
H(x, y, t) = \left( \frac{1}{4\pi t} \right)^{n/2} e^{-\frac{\text{dist}^2(x, y)}{4t}} \quad \text{when } M = \mathbb{R}^n.
\]

**\(H(x, y, t) = \sum_j e^{-t\lambda_j} e_j(x) e_j(y)\)** when manifold \(M\) is compact and \(\{\lambda_j\}\) and \(\{e_j\}\) are eigenvalues and eigenfunctions of \(-\Delta_g\) on \(M\).

**No** exact formula for the heat kernel \(H(x, y, t)\) for general manifold \(M\)!
Short Time Asymptotic Expansion of the Heat Kernel $H(x, y, t)$:

$\exists H_i(x, y)$ on $(M \times M) \setminus C(M)$, $C(M) = \{(x, y) | y \in \text{Cut}(x)\}$, such that

$$H(x, y, t) \sim \left(\frac{1}{4\pi t}\right)^{n/2} e^{-\frac{\text{dist}^2(x, y)}{4t}} \sum_{i=0}^{\infty} H_i(x, y) t^i$$

(2)

holds uniformly as $t \to 0$ on compact subsets of $(M \times M) \setminus C(M)$.

**Question:** (Global bounds for the heat kernel $H(x, y, t)$)

Are there $A(\text{dist}(x, y), t)$ and $B(\text{dist}(x, y), t)$ such that

$$A(\text{dist}(x, y), t) e^{-\frac{\text{dist}^2(x, y)}{4t}} \leq H(x, y, t) \leq B(\text{dist}(x, y), t) e^{-\frac{\text{dist}^2(x, y)}{4t}}?$$

(3)

**Remark:** By Cheeger-Yau('81) lower bound comparison Theorem and Davies-Mandouvalos('88) Heat kernel bounds on space form, one has

$$H(x, y, t) \geq H^k(x, y, t) \geq c(n)^{-1} h_n(\text{dist}(x, y), t)$$

where $H^k(x, y, t)$ is the heat kernel of space form with $\text{Ric} = -k$ and $h_n(r, t)$ is a known function.
Li-Yau Differential Harnack inequality:

\[(Li - Yau'86) \quad \frac{|\nabla u|^2}{u^2} - \alpha \frac{u_t}{u} \leq \frac{n\alpha^2 k}{2(\alpha - 1)} + \frac{n\alpha^2}{2t}, \quad \forall \alpha > 1.\]

When \((M, g)\) with nonnegative Ricci curvature, the sharp estimate:

\[\frac{|\nabla u|^2}{u^2} - \alpha \frac{u_t}{u} \leq \frac{n}{2t}.\]

\[(Davies'89) \quad \frac{|\nabla u|^2}{u^2} - \alpha \frac{u_t}{u} \leq \frac{n\alpha^2 k}{4(\alpha - 1)} + \frac{n\alpha^2}{2t}, \quad \forall \alpha > 1.\]

Harnack inequality:

Let \(u(x, t)\) be a positive solution of the heat equation (1), then \(\forall \alpha > 1,

\[u(x_1, t_1) \leq u(x_2, t_2) \left(\frac{t_2}{t_1}\right)^{\frac{n\alpha}{2}} \cdot \exp \left(\frac{\alpha \text{dist}^2(x, y)}{4(t_2 - t_1)} + \frac{n\alpha k}{4(\alpha - 1)}(t_2 - t_1)\right).\]

where \(x_1, x_2 \in M\) and \(0 < t_1 < t_2 < \infty\).
Li-Yau’s Bound estimates of $H(x, y, t)$

- **Upper bound of $H(x, y, t)$**: $\forall \delta > 0$,

$$H(x, y, t) \leq C(\delta, n)V_x^{-\frac{1}{2}}(\sqrt{t})V_y^{-\frac{1}{2}}(\sqrt{t}) \cdot \exp \left(- \frac{dist^2(x, y)}{(4 + \delta)t} + C_1(n)\delta kt \right).$$

where $V_x(R) = \text{Vol}(B_x(R))$ and $C(\delta, n) \sim \exp(\frac{C}{\delta})$ as $\delta \to 0$.

- **Lower bound of $H(x, y, t)$ for $\text{Ric}(M) \geq 0$**:

$$H(x, y, t) \geq C^{-1}(\delta, n)V_x^{-\frac{1}{2}}(\sqrt{t})V_y^{-\frac{1}{2}}(\sqrt{t}) \cdot \exp \left(- \frac{dist^2(x, y)}{(4 - \delta)t} \right).$$

**Remark**: By a slight modified proof of Li-Yau, one could improve as

$$H(x, y, t) \leq C(n)V_x^{-\frac{1}{2}}(\sqrt{\delta t})V_y^{-\frac{1}{2}}(\sqrt{\delta t}) \cdot \exp \left(- \frac{dist^2(x, y)}{(4 + \delta)t} + C_1(n)\delta kt \right).$$
Motivation to improve Li-Yau type estimates

- Short time behavior of the heat kernel $H(t, x, y)$:

\[ H(t, x, x) \sim t^{-n/2}(a_0 + a_1 t + a_2 t^2 + \cdots), \text{ as } t \searrow 0 \]

which suggests

\[ \frac{-u_t}{u} \sim \frac{n}{2t}, \text{ as } t \searrow 0 \]

- Long time asymptotic behavior of upper bound for $\varphi(t)$:
  1. Davies’ estimates suggest the lowest upper bound for $\varphi(t)$ may be $nk$ as $t \nearrow \infty$
  2. Yau’s gradient estimates for positive harmonic functions on manifolds with negative Ricci lower bound:

\[ \frac{|\nabla u|^2}{u^2} \leq (n - 1)k \]

(3) Direct computation for the heat kernel $H(t, x, y)$ on hyperbolic spaces suggest the lowest upper bound for $\varphi(t)$ will be at least $(n - 1)k$ too.
Li-Yau type Differential Harnack inequality

**Theorem:** (Li-X. ’11) Let $B_{2R}$ be a geodesic ball with $\text{Ricci}(B_{2R}) \geq -k$. Let $f = \ln u$, then we get the following Li-Yau type gradient estimate in $B_R$

$$
\sup_{B_R} (|\nabla f|^2 - \alpha f_t - \varphi)(x, t) \leq \frac{nC}{R^2} + \frac{nC \sqrt{k}}{R} \coth(\sqrt{k} \cdot R) + \frac{n^2 C}{R^2 \tanh(kt)}.
$$

where $\alpha(t) = 1 + \frac{\sinh(kt) \cosh(kt) - kt}{\sinh^2(kt)}$ and $\varphi(t) = \frac{nk}{2} \left[ \coth(kt) + 1 \right]$. Moveover, if $\text{Ric}(M) \geq -k$ on the complete manifold, then

$$
|\nabla f|^2 - (1 + \frac{\sinh(kt) \cosh(kt) - kt}{\sinh^2(kt)})f_t \leq \frac{nk}{2} \left[ \coth(kt) + 1 \right]. \quad (4)
$$

**Remark:**

$\alpha(t) \to 1$ and $\varphi(t) \to \frac{n}{2t}$ as $t \searrow 0$,
$\alpha(t) \to 2$ and $\varphi(t) \to nk$ as $t \nearrow \infty$. 

Parabolic Harnack inequalities for positive solutions

**Theorem:** (Li-X. ’11) For $\forall x_1, x_2 \in M, 0 < t_1 < t_2 < \infty$,

$$\frac{u(x_1, t_1)}{u(x_2, t_2)} \leq A_1(t_1, t_2) \cdot \exp \left[ \frac{\text{dist}^2(x_2, x_1)}{4(t_2 - t_1)} (1 + A_2(t_1, t_2)) \right]$$

where $\text{dist}(x_1, x_2)$ is the distance between $x_1$ and $x_2$,

$$A_1 = \left( \frac{e^{2kt_2} - 2kt_2 - 1}{e^{2kt_1} - 2kt_1 - 1} \right)^{n/4}$$

and

$$A_2(t_1, t_2) = \frac{t_2 \coth(kt_2) - t_1 \coth(kt_1)}{t_2 - t_1}.$$

**Sketch of Proof:** One integrates the following Hamilton-Jacobi inequality

$$f_t \geq -\frac{1}{\alpha} (\phi(t) - |\nabla f|^2),$$

which comes from (4), along the curve $\eta(s) = (\gamma(s), (1 - s)t_2 + st_1)$, where $\gamma$ is a shortest geodesic joining $x_1$ and $x_2$. 
On-diagonal upper bound of $H(x, y, t)$:

**Theorem:** (X. ‘13) For any $R > 0$, we have

$$H(x, y, t) \leq V_x^{-\frac{1}{2}}(R)V_y^{-\frac{1}{2}}(R)A_1^2\left(\frac{t}{2}, \frac{t}{2} + \delta\left(\frac{t}{2}\right)\right)\exp\left[\frac{R^2}{2\delta(t)}\left(2 + A_2\left(\frac{t}{2}, \frac{t}{2} + \delta\left(\frac{t}{2}\right)\right)\right)\right].$$

One can obtain different on-diagonal upper bound of the heat kernel by different choice of $\delta(t)$ and $R$:

**Case 1:** $\delta(t) = (2t)^2 \land 1 \triangleq \min\{(2t)^2, 1\}$ and $R^2 = \delta\left(\frac{t}{2}\right) = t^2 \land 1$,

$$H(x, y, t) \leq V_x^{-\frac{1}{2}}(t \land 1)V_y^{-\frac{1}{2}}(t \land 1)A_{on}(t)\exp(B_{on}(t)), \quad (5)$$

where $A_{on}(t)$ and $B_{on}(t)$ are bounded functions such that: $A_{on}(t) \sim 1$ as $t \to 0$, $A_{on}(t) \sim \exp\left[\frac{nk}{2}\right]$ as $t \to \infty$, $B_{on}(t) \sim 1 + \frac{k(t+t^2)}{6}$ as $t \to 0$, $B_{on}(t) \sim \frac{3}{2}$ as $t \to \infty$. 

Case 2: $\delta(t) = (2t)^2 \wedge t \overset{\Delta}{=} \min\{(2t)^2, t\}$ and $R^2 = \delta\left(\frac{t}{2}\right) = t^2 \wedge t$, 

$$H(x, y, t) \leq V_x^{-\frac{1}{2}}(t \wedge \sqrt{t})V_y^{-\frac{1}{2}}(t \wedge \sqrt{t})A_{on}(t) \exp(B_{on}(t)), \quad (6)$$

where $A_{on}(t)$ and $B_{on}(t)$ are smooth functions such that: $A_{on}(t) \sim 1$ as $t \to 0$, $A_{on}(t) \sim \exp\left[\frac{nkt}{2}\right]$ as $t \to \infty$, $B_{on}(t) \sim 1 + \frac{k(t+t^2)}{6}$ as $t \to 0$, $B_{on}(t) \sim 2$ as $t \to \infty$.

Case 3: $\delta(t) = 2t \wedge 1 \overset{\Delta}{=} \min\{2t, 1\}$ and $R^2 = \delta\left(\frac{t}{2}\right)$,

$$H(x, y, t) \leq V_x^{-\frac{1}{2}}(\sqrt{t} \wedge 1)V_y^{-\frac{1}{2}}(\sqrt{t} \wedge 1)A(t) \exp(B(t)), \quad (7)$$

where $A(t) \sim 2^{n/2}$ as $t \to 0$, $A(t) \sim \exp\left[\frac{nk}{2}\right]$ as $t \to \infty$, $B(t) \sim 1 + \frac{kt}{3}$ as $t \to 0$, $B(t) \sim \frac{3}{2}$ as $t \to \infty$. 

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if we further assume that \( \inf_{x \in M} V_x(1) \geq \epsilon > 0 \) for some constant \( \epsilon > 0 \), we have

\[
H(x, y, t) \leq \begin{cases} 
C_1 t^{-n/2}, & t \leq 1, \\
C_2, & t \geq 1.
\end{cases}
\]

From A Theorem of Davies-Pang ‘89. We have

\[
H(x, y, t) \leq C \max \left\{ t^{-n/2} \left( 1 + \frac{d(x, y)}{\sqrt{t}} \right)^n, 1 \right\} \exp \left[ -\frac{d^2(x, y)}{4t} \right] \tag{8}
\]

where \( C \) depends on \( n, k, \epsilon \) only.
Off-diagonal upper bound of $H(x, y, t)$:

**Theorem:** (X. ’13): Assume $d^2(x, y) > t^2 \land 1$, we have the following off-diagonal upper bound of the heat kernel

$$H(x, y, t) \leq V_x^{-\frac{1}{2}}(t \land 1)V_y^{-\frac{1}{2}}(t \land 1)A_{off}(t) \exp \left[ -\frac{d^2(x, y)}{4t} + B_{off}(t) + C_{off}(t)d^2(x, y) \right], \quad (9)$$

where $A_{off}(t)$, $B_{off}(t)$ and $C_{off}(t)$ are bounded functions such that:

- $A_{off}(t) \sim 1$ as $t \to 0$, $A_{off}(t) \sim e^{nk}$ as $t \to \infty$, $B_{off}(t) \sim 1$ as $t \to 0$,
- $B_{off}(t) \sim \frac{5}{4}$ as $t \to \infty$, and $C_{off}(t) \sim \frac{5}{4}$ as $t \to 0$, $C_{off}(t) \sim 0$ as $t \to \infty$.

And

$$H(x, y, t) \leq V_x^{-\frac{1}{2}}(t \land \sqrt{t})V_y^{-\frac{1}{2}}(t \land \sqrt{t})A_{off}(t) \exp \left[ -\frac{d^2(x, y)}{4t} + B_{off}(t) + C_{off}(t)d^2(x, y) \right], \quad (10)$$

where $A_{off}(t)$, $B_{off}(t)$ and $C_{off}(t)$ are smooth functions such that:

- $A_{off}(t) \sim 1$ as $t \to 0$, $A_{off}(t) \sim e^{nkt}$ as $t \to \infty$, $B_{off}(t) \sim 1$ as $t \to 0$,
- $B_{off}(t) \sim \frac{5}{4}$ as $t \to \infty$, and $C_{off}(t) \sim \frac{5}{4}$ as $t \to 0$, $C_{off}(t) \sim 0$ as $t \to \infty$. 

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Upper bound estimate for Heat kernel $H(x, y, t)$

**Theorem: (X. ‘13)** Let $(M, g)$ be a complete Riemannian manifold with $Ric(M) \geq -k$, $k \geq 0$. Let $H(x, y, t)$ be the heat kernel of $M$, then

\[
H(x, y, t) \leq V_x^{-\frac{1}{2}}(t \wedge 1)V_y^{-\frac{1}{2}}(t \wedge 1)A(t) \times \exp \left[ -\frac{d^2(x, y)}{4t} + B(t) + C(t)d^2(x, y) \right],
\]

where $A(t) = \max\{A_{on}(t), A_{off}(t)\}$, $B(t) = \max\{B_{on}(t) + \frac{t^2}{4t}, A_{off}(t)\}$ and $C(t) = C_{off}(t)$ are positive bounded functions such that:

\[
A(t) \sim \begin{cases} 
1, & \text{as } t \to 0, \\
e^{nk}, & \text{as } t \to \infty.
\end{cases}
\]

\[
B(t) \sim \begin{cases} 
1, & \text{as } t \to 0, \\
\frac{3}{2}, & \text{as } t \to \infty.
\end{cases}
\]

\[
C(t) \sim \begin{cases} 
\frac{5}{4}, & \text{as } t \to 0, \\
0, & \text{as } t \to \infty.
\end{cases}
\]
New lower bounds of the heat kernel

**Theorem:** (Li-X. ’11) Let $M$ be a complete (or compact with convex boundary) Riemannian manifold possibly with $\text{Ricci}(M) \geq -k$. Let $H(x, y, t)$ be the (Neumann) heat kernel. Then for all $x, y \in M$ and $t > 0$,

$$H(x, y, t) \geq (4\pi t)^{-\frac{n}{2}} \frac{(2kt)^{\frac{n}{2}}}{(2e^{2kt} - 2 - 4kt)^{\frac{n}{4}}} \cdot \exp \left[ - \frac{d^2(x,y)}{4t} \left( 1 + \frac{kt \coth(kt) - 1}{kt} \right) \right].$$

In particular when $\text{Ricci}(M) \geq 0$, we have

$$H(x, y, t) \geq (4\pi t)^{-\frac{n}{2}} \exp \left[ - \frac{d^2(x,y)}{4t} \right].$$

**Theorem:** (X. ’13) Lower bound of $H(x, y, t)$ for $\text{Ric}(M) \geq 0$:

$$H(x, y, t) \geq \tilde{A}(t)V_x^{-\frac{1}{2}}(t)V_y^{-\frac{1}{2}}(t) \cdot \exp \left( - \frac{\text{dist}^2(x,y)}{4t} - \tilde{B}(t)\text{dist}^2(x,y) \right).$$


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Thank you for attention!