Second order variation and the logarithmic heat kernel

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The heat kernel

$$\frac{\partial}{\partial t}u_t = \frac{1}{2}\Delta u_t,$$
$$u_0 = f$$

If a heat source is placed at x, the spike decays quickly and flats out. The heat is moved around but not lost. A fundamental solution at x satisfies $\lim_{t\to 0} p(t,x,y) = \delta_x(y)$. The heat kernel is the minimal positive fundamental solution which can be obtained from the integral L^2 kernel:

$$u_t(x) = \int_M f(y)p(t,x,y)dy.$$

Through Chapman-Kolmogorov equation, $p(t,x,y)$ can be defined for all x, y and any $t > 0$.

Global Estimates

Gradient estimates for solutions non-compact spaces are relevant for simply just justify the conservation law:

$$\frac{d}{dt}\int_D u_t \, dvol = \int_D \frac{1}{2}\Delta u_t \, dvol = \frac{1}{2}\int_{\partial D} \nabla u_t \cdot \vec{n} \, dS.$$

They involve the geometry globally. If D is compact, need conditions so $|\nabla u|$ decays sufficiently fast, in x, for it to be integrable.
Global estimates: [3,5]

Small time estimates

When the time is small, the heat kernel should behaves like an Euclidean kernel. Hence we expect Gaussian upper lower bounds, and similar bounds for $\nabla \log p(t, x, y)$ and $\nabla^2 \log p(t, x, y)$.
However, a Brownian motion makes large deviations, e.g. positive fundamental solution may not be unique for some manifolds.
In any case, all results are obtained so far are subjet to some conditions: Manifold is compact, bounds on the Ricci curvature, or bounded geometry.

Conquest. Obtain small time estimates without any curvature restrictions.

Sample estimates we are after

$x, y \in K$ compact, $t \in (0,1]$.

$$|\nabla_x \log p(t,x,y)|_{T_xM} \leq C(K)\left(\frac{1}{\sqrt{t}} + \frac{d(x,y)}{t}\right) \quad (1)$$

$$\left|\nabla_x^2 \log p(t,x,y)\right|_{T_xM\otimes T_xM} \leq C(K)\left(\frac{d^2(x,y)}{t^2} + \frac{1}{t}\right) \quad (2)$$

$$\lim_{t\downarrow 0} \sup_{x\in\tilde{K}} \left| t\nabla_x \log p(t,x,y) + \nabla_x\left(\frac{d^2(x,y)}{2}\right)\right|_{T_xM} = 0, \quad (3)$$

$$\lim_{t\downarrow 0} \sup_{x\in\tilde{K}} \left| t\nabla_x^2 \log p(t,x,y) + \nabla_x^2\left(\frac{d^2(x,y)}{2}\right)\right|_{T_xM\otimes T_xM} = 0 \quad (4)$$

$\tilde{K} \subset M \setminus \mathrm{Cut}(y)$ is a compact set.

These estimates are known under restrictions or on compact, e.g. Sheu91, Hamilton93, Malliavin-Stroock 96, Hsu99, Aida04, Li-Yau86, extended reference in [1].

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The caveat of passing from compact space to a non-compact space

Estimates were obtained under curvature restriction. To get over this we must find an vantage point of that compact manifolds. One can try to localise the problem Two standard methods of localisation do not work well.

- Exit time of the Brownian motion from a relatively compact open set with smooth boundary is not continuous with respect to its initial condition.
- the explosion problem is not local
- Geodesic balls may not have smooth boundaries.
- Modify the Riemannian metric with a function f blowing up on the boundary of a relatively compact set with smooth boundary? The resulting manifold D is complete, not compact. Higher order derivatives of the function f cannot be easily controlled.

Second order stochastic variations

Our techniques relies on construct compact embeddings, and bootstrap by obtaining quantitative estimates for the difference of the heat kernel and its logarithmic derivatives on the exhaustion with that on the whole manifold.
One needs to be careful, as Brownian paths can shoot out quickly.
We need a formula for $\nabla^2 \log p(t,x,y)$ in which the cut off processes appear in a suitable format.
For this we introduce a second oder stochastic variation on the orthonormal frame bundle, which allows us to prescribe the second order derivatives of the variation.

Varadhan Estimates and large deviation

For any $x, y \in M$,

$$\lim_{t \downarrow 0} t \log p(t, x, y) = -\frac{d(x, y)^2}{2}. \tag{5}$$

Azencott, Molchanov
Connected bounded open set $D \supseteq K$ with smooth boundary,

$$\lim_{t \downarrow 0} t \log \mathbb{P}_x(\tau_D < t) = -\frac{d(x, \partial D)^2}{2}, \quad \forall\, x \in K. \tag{6}$$

$\tau_D := \inf\{t > 0; X_t \notin D\}$and $d(x, \partial D) := \inf_{z \in \partial D} d(x, z)$.

Compact approximations

The following is joint work with Chen and Wu, [1].
We being by constructing a family of bounded connected open sets $\{D_m\}_{m=1}^{\infty}$ with **quantitative** cut-off properties.

One construct a compact Riemannian manifold $\tilde{M}_m$ such that D_m is isometrically embedded into $\tilde{M}_m$ as an open set.

Lemma 1. Suppose that K is a compact subset of M and $L > 1$ is a positive number. Then for sufficiently large m, there exists a positive number $t_0 = t_0(K, L, m)$ such that for every $t \in (0, t_0]$,

$$\sup_{x,y \in K} \left| p(t,x,y) - p_{\tilde{M}_m}(t,x,y) \right| \leq e^{-\frac{L}{t}}. \tag{7}$$

Quantitative comparison theorems

[Chen, L , Wu 21]

$0 < s \le \frac{t}{2}$ and $0 < t \le t_0$, we have

$$\sup_{x,y\in K} \sup_{z\in D_{m_0}} \left| \frac{p(t-s,x,z)}{p(t,x,y)} - \frac{p_{\tilde M_m}(t-s,x,z)}{p_{\tilde M_m}(t,x,y)} \right| \le 2e^{-\frac{4L}{t}}. \quad (8)$$

$$\sup_{x,y\in K} \left| \nabla_x \log p(t,x,y) - \nabla_x \log p_{\tilde M_m}(t,x,y) \right|_{T_x M} \le C(m) e^{-\frac{L}{t}} \quad (9)$$

At this stage we use a suitable second order derivative formula to obtain Hessian estimates $\nabla^2 \log p_t$.

$$\sup_{x,y\in K} \left| t\nabla_x^2 \log p(t,x,y) - t\nabla_x^2 \log p_{\tilde M_m}(t,x,y) \right|_{T_x M \otimes T_x M} \le C(m) e^{-\frac{L}{t}}$$

Motivation

- Study probability measure on loop subspace of $C([0,1];M)$. The classical problems are: do they exists, how do they behave at infinity?
- The decay problem can be solved by Poincare inequalities.
- Define a Ornstein-Uhlenbeck like process on the loop space.
- Even Talagrand's conjecture can be sometimes solved with such estimates. The conjecture is:

$$\sup_{\|f\|_{L^1}=1} \gamma_n(\{T_s f \geq t\}) \leq C_s \frac{1}{t\sqrt{\log t}}.$$

Ball, Barthe, Bednorz, Oleszkiewicz, and Woff.

Hypo-elliptic Case

To make connection with the community on Sub-Riemannian geometry, let

$$\mathcal{L} = \frac{1}{2} \sum_i (X_i)^2 + X_0$$

be a hypo-elliptic operator. Then there exists a smooth kernel $p(t, x, y)$ such that

$$P_t f(x) = \int_M f(y) p(t, x, y) dy.$$

To condition the Markov process from x_0 to y_0 in time 1, it is reasonable to assume there exists a controllable path between them. So it is natural to assume the strong Hörmander's condition on $\mathcal{L}$. In this case

$$p(t, x, y) > 0.$$

The hypo-elliptic bridge

Assume the strong Hörmander's condition. The $\mathcal{L}$-diffusion x_t conditioned process has generator

$$\mathcal{L} + \nabla \log p(1-t, x, y), \qquad t < 1.$$

It is the pinned process solving:

$$dy_t = X_i(y_t) \circ dB_t^i + \nabla \log p(1-t, x, y_t) dt.$$

$$\lim_{t \to 1} y_t = 1, \qquad \text{almost surely?}$$

If so, this is a (successful) hypo-elliptic bridge.
The finite dimensional distribution then determine a probability measure on the loop (pinned path space).

Strong Hörmander's condition

Theorem (ECP 2016). Suppose that the $\mathcal{L}$ is conservative and satisfies the strong Hömander's condition, $\mathcal{L}^*\mu = 0$ has a solution. Let $\hat{L}$ be the adjoint w.r.t. μ, suppose it is conservative. (1) Then y_t is a hypo-elliptic bridge.
(2) Furthermore, if $\mathcal{L}$ satisfies a two step Hörmandr's condition and M is compact, then

$$\int_0^1 \sqrt{\mathbb{E}|\nabla \log p(1-s, y_s, z)|^2} ds < \infty$$

and $y_t, t \leq 1$ is a semi-martingale.
The problem is open for the general case.
Te proof of part (2) , under the two step Hörmander condition, uses a gradient estimate of Cao-Yau 92:
$\sum_i \langle |\nabla \log u, X_i\rangle|^2 \leq \delta \frac{\partial}{\partial t} \log u + \frac{C}{t} + C$.

Canonical Brownian motion

Consider a family of horizontal vector fields H_i on the orthonormal frame bundle OM.

$$du_t = \sum_{i=1}^{n} H_i(u_t) \circ dB_t^i, \qquad \pi(u_0) = x_0.$$

Eells-Elworthy, Malliavin, $\pi(u_t)$ is a Brownian motion.
c.f. Talk by Fang and Perruchaud.

The other construction is given by isometric embeddings, the resulting process is extrinsic, has extra noise, unless the manifold is parallelable. This is the gradient Brownian motion.

Stochastic Variation à la Bismut

Let $h \in L^{2,1}(\mathbb{R}^n)$ be a Cameron-Martin vector and

$$\hat{B}_t^\epsilon = \int_0^t e^{-\epsilon\Gamma_s} dB_s + \epsilon \int_0^t (h'(s) + \frac{1}{2}\mathrm{ric}_{U_s} h(s)) ds.$$

$$du_t = \sum_{i=1}^n H_i(u_t) \circ dB_t^{i,\epsilon}, \qquad \pi(u_0) = x_0.$$

Then we expect that variation of the initial condition of the solution is the same as that given by the variation in noise.

$$\Gamma_t^h = \int_0^t R(\circ dB_s, h(s)).$$

This leads to Bismut's formula for $\nabla \log p(t, x, y)$: with right hand side involving the Brownian bridge which depends also on $\nabla \log p$ (so it is apparent how to use it for obtaining estimates for $\nabla \log p(t, x, y)$)

Integration by part

Crucially,

$$\frac{\partial}{\partial \varepsilon}|_{\varepsilon=0}\pi(U_t^\varepsilon) = U_t h(t).$$

With this method, Driver, c.f. Bismut, obtained an integration by part formula:

$$\mathbb{E}dF(U.h) = \mathbb{E}F\int_0^t \langle h'(s) + \frac{1}{2}\mathrm{ric}_{U_s}h(s), dB_s\rangle.$$

If F depends only on one time, $F(\sigma) = f(\sigma_t)$, one has

$$\mathbb{E}df(U_t h_t) = \mathbb{E}F(x_t)\int_0^t \langle h'(s) + \frac{1}{2}\mathrm{ric}_{U_s}h(s), dB_s\rangle.$$

A formula equivalent to Integration by parts

A differentiation formula is given in [Li92], which was shown [Elworthy-L.96] to be equivalent to Integration by parts formula on compact. We employ the methods in [Li92] to prove an intrinsic version:

$$du_t = H(u_t) \circ dB_t, \qquad \pi(u_t) = x_t,$$

$$dx_t = u_t \circ dB_t \qquad T\pi(u_t e) = u_t e$$

$$f(x_T) = P_t f(x_0) + \int_0^T dP_{T-s} f(T\pi \circ H(u_s) dB_s$$

$$= P_t f(x_0) + \int_0^T dP_{T-s} f(u_s \circ dB_s).$$

Note: $dP_t f(v) = \mathbb{E} df(W_t(v))$, as noted in Airault, c.f. Maliiavin, Elworthy,

$$\frac{1}{T}\mathbb{E} f(x_T) \int_0^T \langle u_s dB_s, W_s(v) \rangle = \frac{1}{T}\mathcal{E} \int_0^T \mathbb{E} dP_{T-s} f(W_s(v)) ds$$

Second order derivatives

In Bismut's approach, the key is $\frac{\partial}{\partial\varepsilon}|_{\varepsilon=0}\pi(U_t^\varepsilon) = U_t h(t)$. However $\frac{\partial^2}{\partial\varepsilon^2}|_{\varepsilon=0}\pi(U_t^\varepsilon) \neq 0$ as long as $h(t) \not\equiv 0$. and is not controllable. For the first order variation, one does not need to work on TOM. We introduce a new method with prescribed derivative. The method we discuss next can be adapted to solve a number of other problems.
On the tangent space of the orthonormal frame bundle, any vector splits into a horizontal part and a vertical part. The vertical and horizontal part interact through the curvatures.

$$\varpi_t^\varepsilon := \varpi\left(\frac{\partial}{\partial\varepsilon}U_t^\varepsilon\right), \qquad \theta_t^\varepsilon := \theta\left(\frac{\partial}{\partial\varepsilon}U_t^\varepsilon\right).$$

We want

$$\eta_s := \frac{\partial\theta_s^\varepsilon}{\partial\varepsilon}\Big|_{\varepsilon=0} = 0.$$

Intrinsic Connection on OM

At this stage we must choose a connection on the orthonormal frame bundle. One can use the connection associated with the Horizontal frames.

Second order variation [Chen-Li-Wu 2021]

We make a variation of the initial point of the Brownian motion plus a variation of the noise of the second order:

$$B_t^{\varepsilon,h} := B_t + \epsilon \int_0^t h'(s) ds + \frac{\epsilon^2}{2} \int_0^t \Gamma_t^h h'(t)\, ds,$$

$$d\tilde{B}_t^{\varepsilon,h} = G_t^{\varepsilon,h} \circ dB_t^{\epsilon,h}$$

$$G_t^{\varepsilon,h} := \exp\left(-\varepsilon \Gamma_t^h. - \frac{\varepsilon^2}{2} \Gamma_t^{(2),h}\right),$$

$$\begin{aligned}\Gamma_t^{(2),h} := & \int_0^t U_s^{-1} \nabla \mathbf{R}_{\pi(U_s)}\big(U_s h(s), U_s \circ \mathrm{d}B_s, U_s h(s)\big) \\ & - \int_0^t \Gamma_s^h \mathrm{R}_{U_s}(\circ \mathrm{d}B_s, h(s)) \\ & + \int_0^t \mathrm{R}_{U_s}(h'(s), h(s))\mathrm{d}s + \int_0^t \mathrm{R}_{U_s}\big(\circ \mathrm{d}B_s, \Gamma_s^h h(s)\big).\end{aligned}$$

Let $\xi(\varepsilon)$, $\varepsilon \in (-1,1)$, be a geodesic with $\xi(0) = x$. Now all wishes come true, in addition:

$$\frac{D}{\partial\varepsilon}\Big|_{\varepsilon=0}\left(\frac{\partial X_t^\varepsilon}{\partial\varepsilon}\right) = U_t \Gamma_t h(t).$$

Let M_t^ε be the exponential martingale, $\xi(\varepsilon)$ the geodesic variation.

$$M_t^\varepsilon := \exp\left(-\int_0^t \left\langle \varepsilon\Theta_s + \frac{\varepsilon^2}{2}\Lambda_s, \mathrm{d}B_s \right\rangle - \int_0^t \left(\frac{\varepsilon^2}{2}\left|\Theta_s + \frac{\varepsilon}{2}\Lambda_s\right|^2\right)\mathrm{d}s\right)$$

Differentiate

$$P_t f(\xi(\varepsilon)) = \mathbb{E}\Big[f(X_t^{\xi(\varepsilon)})\Big] = \mathbb{E}\Big[f(X_t^{\varepsilon,\xi(\varepsilon)})M_t^\varepsilon\Big], \qquad (10)$$

to obtain the required formula.

Hessian Formula

Proposition (Chen-Li-Wu-2021). Let $x \in M$ and $v \in T_x M$. Then for any $f \in C_b(M)$ and $h \in L^{2,1}(\Omega; \mathbb{R}^n)$ satisfying that $h(0) = U_0^{-1} v$ and $h(t) = 0$ $a.s.$, we have

$$\left\langle \nabla P_t f(x), v \right\rangle_{T_x M} = -\mathbb{E}\left[f(X_t^x) \int_0^t \langle \Theta_s^h, dB_s \rangle \right], \tag{11}$$

where $\Theta_t^h := h'(t) + \frac{1}{2}\mathrm{ric}_{U_t}(h(t))$. Furthermore,

$$\begin{aligned} &\left\langle \nabla^2 P_t f(x), v \otimes v \right\rangle_{T_x M \otimes T_x M} \\ &= \mathbb{E}\left[f(X_t^x) \left(\left(\int_0^t \left\langle \Theta_s^h, \mathrm{d}B_s \right\rangle \right)^2 - \int_0^t \left\langle \Lambda_s^h, \mathrm{d}B_s \right\rangle - \int_0^t \left| \Theta_s^h \right|^2 \mathrm{d}s \right) \right]. \end{aligned} \tag{12}$$

$$\Gamma_t^h := \int_0^t \mathrm{R}_{U_s}(\circ \mathrm{d}B_s, h(s)),$$

$$\Theta_t^h := h'(t) + \frac{1}{2}\mathrm{ric}_{U_t}(h(t)),$$

$$\Lambda_t^h := \Gamma_t^h h'(t) + \frac{1}{2}U_t^{-1}\ \nabla \mathrm{Ric}^\sharp_{X_t}\big(U_t h(t), U_t h(t)\big)$$
$$- \frac{1}{2}\Gamma_t^h\ \mathrm{ric}_{U_t}(h(t)) + \frac{1}{2}\mathrm{ric}_{U_t}\big(\Gamma_t^h h(t)\big).$$

This allow to extend to any complete Riemannian manifolds by choosing a suitable h vanishing on $s > \frac{t}{2}$.

$$\big\langle \nabla^2 P_t f(x), v \otimes v \big\rangle_{T_xM\otimes T_xM}$$
$$= \mathbb{E}_x\Big[\Big(\big(\int_0^t \langle \Theta_s^h, \mathrm{d}B_s\rangle\big)^2 - \int_0^t \langle \Lambda_s^h, \mathrm{d}B_s\rangle - \int_0^t \big|\Theta_s^h\big|^2 \mathrm{d}s\Big)$$
$$f(X_t^x)\mathbf{1}_{\{t<\zeta(x)\}}\Big].$$

To compare

Extrinsic formula from Elworthy- L. [2(1)], using SDE

$$\mathrm{Hess} P_t f(x_0)(v_1, v_2) = \frac{4}{t^2}\mathbb{E}\left\{ f(x_t) \int_{\frac{t}{2}}^{t} \langle Y(x_s)u_s, dB_s\rangle \int_0^{\frac{t}{2}} \langle Y(x_s)v_s, dB_s\rangle \right\}$$
$$+ \frac{2}{t}\mathbb{E}\left\{ f(x_t) \int_0^{\frac{t}{2}} \langle DY(x_s)(u_s)(v_s), dB_s\rangle \right\}$$
$$+ \frac{2}{t}\mathbb{E}\left\{ f(x_t) \int_0^{\frac{t}{2}} \langle Y(x_s)\nabla TF_s(v_1, v_2), dB_s\rangle \right\}.$$

Intrinsic version of above is obtained in Aranudon, Planck, Thalmaier Also from Li'16 [3] : Hybrid formula is obtained :

$$\mathrm{Hess}(P_t^h f)(v_2, v_1) = \mathbb{E}[\nabla df(W_t(v_2), W_t(v_1))] + \mathbb{E}\left[df(W_t^{(2)}(v_1, v_2)) \right],$$

Hybrid fromula

From [3]

$$\mathrm{Hess} P_t^h f(v_1, v_2) = \frac{4}{t^2}\mathbb{E}\left[f(x_t) \int_{t/2}^{t} \langle d\{x_s\}, W_s(v_1)\rangle \int_0^{t/2} \langle d\{x_s\}, W_s(v_2)\rangle \right] + \frac{2}{t}\mathbb{E}\left[f(x_t) \int_0^{t/2} \langle d\{x_s\}, W_s^{(2)}\rangle \right],$$

This is good for obtaining global estimates. It does not work well for our purpose.

$$DW_t^{(2)}(v_1, v_2) = (-\frac{1}{2}\mathrm{Ric}^\sharp + (\nabla^2 h)^\sharp)\left(W_t^{(2)}(v_1, v_2)\right)dt + \frac{1}{2}\Theta^h(W_t(v_2))(W_t(v_1))dt + \mathcal{R}(d\{x_t\}, W_t(v_2))W_t(v_1).$$

The Θ^h in the last formula is: For $v_1, v_2, v_3 \in T_{x_0}M$,

$$\langle \Theta(v_2)v_1, v_3\rangle = \left(\nabla_{v_3}\mathrm{Ric}^\sharp\right)(v_1, v_2) - \left(\nabla_{v_1}\mathrm{Ric}^\sharp\right)(v_3, v_2) - \left(\nabla_{v_2}\mathrm{Ric}^\sharp\right)(v_1, v_3),$$

$$\Theta^h(v_2, v_1) = \frac{1}{2}\Theta(v_2)(v_1) + \nabla^2(\nabla h)(v_2, v_1) + \mathcal{R}(\nabla h, v_2)(v_1). \tag{13}$$

Looking forward

- Analysis on loop space, with Chen and Wu.
- Sub-elliptic and ...

The talk is based on

1. Logarithmic heat kernels: estimates without curvature restrictions, Chen, Li, Wu, 2021
2. (i) Elworthy and L. Formulae for the derivatives of heat semigroups. 1994 (ii) A class of Integration by parts formulae in stochastic analysis I.
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4. N. Gozlan, L., M. Madiman, C. Roberto, and P. M. Samson. Log-hessian formula and the talagrand conjecture, arXiv:1907.10896
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