Intertwinings and spectral analysis of diffusion operators

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1. Introduction
2. Intertwinings and Brascamp-Lieb type inequalities
3. The one-dimensional case
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Setting

Consider the Euclidean space $(\mathbb{R}^n, |\cdot|)$ endowed with the probability measure $d\mu(x) \propto e^{-V(x)}dx$, where V is some smooth potential with Hessian matrix $\nabla^2 V$ bounded from below.

Canonical diffusion operator: $Lf = \Delta f - \nabla V \cdot \nabla f$, for which:

- L is (essentially) self-adjoint:

$$\int_{\mathbb{R}^n} f\, Lg\, d\mu = \int_{\mathbb{R}^n} Lf\, g\, d\mu = -\int_{\mathbb{R}^n} \nabla f \cdot \nabla g\, d\mu.$$

- By spectral theorem, we define $P_t := e^{tL}$, $t \geq 0$, a family of symmetric operators on $L^2(\mu)$, satisfying the semigroup property:

$$P_t \circ P_s = P_s \circ P_t = P_{t+s}, \quad \text{and} \quad P_0 = \mathrm{id},$$

and for which μ is invariant:

$$\int_{\mathbb{R}^n} P_t f\, d\mu = \int_{\mathbb{R}^n} f\, d\mu.$$

Probabilistic interpretation

- Markov diffusion process $(X_t)_{t\geq 0}$ on $\mathbb{R}^n$, solution to the Stochastic Differential Equation

$$dX_t = -\nabla V(X_t)dt + \sqrt{2}dB_t,$$

  where $(B_t)_{t\geq 0}$ is a standard Brownian motion on $\mathbb{R}^n$.
- Law of the process coincides with the semigroup: $\mathbb{E}[f(X_t) \mid X_0 = x] = P_t f(x)$.
- The process has (infinitesimal) generator L.
- Invariance: if $X_0 \sim \mu$ then $X_t \sim \mu$ for all $t > 0$.
- Symmetry of the semigroup: if $X_0 \sim \mu$ then for all $T > 0$, the processes $(X_t)_{t\in[0,T]}$ and $(X_{T-t})_{t\in[0,T]}$ have the same law.

Examples

- The Gaussian case:
$$V(x) = \frac{|x|^2}{2},$$
and $\mu = \gamma$ the standard Gaussian distribution $\mathcal{N}(0, I_n)$.
- The Subbotin, or exponential power, distribution:
$$V(x) = \frac{|x|^\alpha}{\alpha},$$
with $\alpha \in [1, \infty]$, the case $\alpha = \infty$ being the uniform measure on the Euclidean unit ball.
- More generally, the log-concave case, i.e. V is convex.
- Heavy-tailed case: Generalized Cauchy:
$$V(x) = \beta \log(1 + |x|^2),$$
with $\beta > n/2$, so that
$$d\mu(x) \propto \frac{1}{(1 + |x|^2)^\beta} \, dx.$$

- The double-well potential:

$$V(x) = \frac{|x|^4}{4} - \frac{|x|^2}{2}.$$

- Product measures perturbed by an interacting term:

$$V(x) = \sum_{k=1}^{n} V_k(x_k) + \sum_{k=1}^{n} \varphi(|x_k - x_{k+1}|).$$

Long-time behaviour

As $t \to \infty$, we have

$$X_t \Longrightarrow X_\infty \quad \text{in law,} \quad \text{where} \quad X_\infty \sim \mu.$$

Many different notions of convergences, and among them:

- Convergence in $L^2(\mu)$ (related to the χ^2 divergence):

$$\mathrm{Var}_\mu(P_t f) := \|P_t f - \mu(f)\|^2_{L^2(\mu)} \underset{t\to\infty}{\longrightarrow} 0,$$

  where $\mu(f) := \int_{\mathbb{R}^n} f \, d\mu$.
- Convergence in $L^1(\mu)$ (related to the total variation distance).
- Convergence in relative entropy (related to the Kullback-Leibler divergence).
- Convergence in Wasserstein (or Kantorovich) distances.

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Poincaré inequality and spectral gap

Proposition

Letting $\lambda > 0$, the following assertions are equivalent:

- *Exponential convergence in $L^2(\mu)$: for all $f \in L^2(\mu)$,*

$$\|P_t f - \mu(f)\|_{L^2(\mu)} \leq e^{-\lambda t} \|f - \mu(f)\|_{L^2(\mu)}.$$

- *Poincaré inequality* ***PI***(λ)*: for all $f \in \mathcal{D}(L)$,*

$$\lambda \operatorname{Var}_\mu(f) \leq \int_{\mathbb{R}^n} f\,(-Lf)\, d\mu.$$

Actually, one has: **PI**$(\lambda) \iff \sigma(-L) \subset \{0\} \cup [\lambda, \infty)$, with $\sigma(-L)$ the spectrum of the non-negative operator $-L$.

The largest λ is called the spectral gap of $-L$ and is denoted λ_1.

Brascamp-Lieb inequality

Theorem (Brascamp-Lieb ('76))

Assume V is strictly convex, i.e. $\nabla^2 V$ is a positive definite matrix. Then for all f smooth enough,

$$\mathrm{Var}_\mu(f) \leq \int_{\mathbb{R}^d} \nabla f \cdot (\nabla^2 V)^{-1} \nabla f \, d\mu. \tag{2.1}$$

- In particular if V is strongly convex, i.e., $\nabla^2 V \geq \lambda I_n$ for some $\lambda > 0$ - an instance of the famous Bakry-Émery curvature-dimension criterion ('85) - then $\mathbf{PI}(\lambda)$ holds.
- Except the Gaussian case, none of the previous examples enter into the strongly convex situation.
- The proof of BL uses a tedious induction on the dimension.
- The inequality is saturated for $f = \nabla V \cdot c$, with $c \in \mathbb{R}^n$ some constant vector.

Classical intertwining

Helffer ('98) revisited the BL inequality, by proposing a simple proof based on an intertwining relation between gradient and operator, the so-called Witten Laplacian approach:

$$\nabla L f = (\mathcal{L} - \nabla^2 V)(\nabla f),$$

with $\mathcal{L} = \mathrm{diag}(L)$ a (diagonal) matrix diffusion operator acting on vector fields and $\nabla^2 V$ is a multiplicative, or 0-order, operator.

At the level of semigroups, we have

$$\nabla P_t f = \mathcal{P}_t^{\nabla^2 V}(\nabla f),$$

with $(\mathcal{P}_t^{\nabla^2 V})_{t \geq 0}$ the Feynman-Kac semigroup acting on vector fields with generator the Schrödinger operator $\mathcal{L} - \nabla^2 V$.

Classical intertwining

In dimension 1, the Feynman-Kac semigroup $(\mathcal{P}_t^{\nabla^2 V})_{t\geq 0}$ admits a simple probabilistic representation: denoting $(X_t^x)_{t\geq 0}$ the process with $X_0 = x \in \mathbb{R}$,

$$P_t^{V''} f(x) = \mathbb{E}\left[f(X_t^x) \exp\left(- \int_0^t V''(X_s^x)\, ds \right) \right].$$

Helffer's proof of the BL inequality

Since we have

$$\nabla(-L)^{-1}f = \int_0^\infty \nabla P_t f \, dt = \int_0^\infty \mathcal{P}_t^{\nabla^2 V}(\nabla f)\, dt = (-\mathcal{L}+\nabla^2 V)^{-1}(\nabla f),$$

Helffer's proof of the BL inequality

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we get after some computations,

$$\mathrm{Var}_\mu(f) = \int_0^\infty \int_{\mathbb{R}^n} \nabla f \cdot \nabla P_t f \, d\mu\, dt$$

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where we used the following inequality, to understand in the sense of self-adjoint operators: $(-\mathcal{L}+\nabla^2 V)^{-1} \leq (\nabla^2 V)^{-1}$.

A new intertwining

Question: how to correct the lack of (strong) convexity in the previous examples ?

Idea: to introduce a weight in the previous intertwining.

Letting $x \in \mathbb{R}^n \to A(x) \in GL_n(\mathbb{R})$ be a smooth mapping seen as a weight, we have

$$A \nabla L f = A (\mathcal{L} - \nabla^2 V) (A^{-1} A \nabla f)$$

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$$\begin{aligned} A\nabla Lf &= A(\mathcal{L} - \nabla^2 V)(A^{-1} A\nabla f) \\ &= \underbrace{\left(\mathcal{L} + 2A\nabla(A^{-1}) \cdot \nabla\right)}_{=:\mathcal{L}_A} (A\nabla f) \\ &\quad - \underbrace{\left(A\nabla^2 V A^{-1} - A\mathcal{L}(A^{-1})\right)}_{=:M_A} (A\nabla f) \end{aligned}$$

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A new intertwining

- $\mathcal{L}_A$ is a (non-diagonal) matrix diffusion operator acting on vector fields, and M_A is 0-order.
- The scalar product of interest on vectors fields is $L^2\left((A\,A^T)^{-1}, \mu\right)$, so that $-\mathcal{L}_A$ is (essentially) self-adjoint and non-negative as soon as

$$A^{-1}\,M_A\,A = \nabla^2 V - \mathcal{L}(A^{-1})\,A,$$

is a symmetric matrix which is bounded from below.

- In terms of semigroups, the intertwining with weight A means that

$$A\,\nabla P_t f = \mathcal{P}_{t,A}^{M_A}\,(A\,\nabla f),$$

with $(\mathcal{P}_{t,A}^{M_A})_{t\geq 0}$ the Feynman-Kac semigroup acting on vector fields, associated to the operator $\mathcal{L}_A - M_A$.

A new intertwining

In dimension 1, the intertwining with weight a is nothing but a composition of the classical intertwining with Doob's $1/a$-transform: "we multiply inside by $1/a$ and divide outside by $1/a$":

$$(P_t f)'(x) \quad = \quad \mathbb{E}\left[f'(X_t^x) \exp\left(- \int_0^t V''(X_s^x)\, ds \right) \right]$$

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where $(X_t^{(a)})_{t\geq 0}$ is the diffusion process with generator L_a and $(M_t^{(a)})_{t\geq 0}$ is the Girsanov martingale

$$M_t^{(a)} = \frac{a(X_{a,t}^x)}{a(x)} \exp\left(- \int_0^t \frac{L_a(a)}{a} (X_{a,s}^x)\, ds \right)$$

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A new intertwining

so that the intertwining with weight a rewrites as

$$a\,(P_t f)'(x) = \mathbb{E}\left[(af')(X_{a,t}^x)\,\exp\left(-\int_0^t (V'' - a\,L(1/a))(X_{a,s}^x)\,ds\right)\right].$$

Generalized BL inequality

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Generalized BL inequality

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\mathrm{Var}_\mu(f) &= \int_0^\infty \int_{\mathbb{R}^n} \nabla f \cdot \nabla P_t f \, d\mu \, dt \\
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&= \int_0^\infty \int_{\mathbb{R}^n} A \nabla f \cdot (A A^T)^{-1} \mathcal{P}_{t,A}^{M_A} (A \nabla f) \, d\mu \, dt
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&\leq \int_{\mathbb{R}^n} A \nabla f \cdot (A A^T)^{-1} \, M_A^{-1} \, A \nabla f \, d\mu \\
&= \int_{\mathbb{R}^n} \nabla f \cdot \left(\nabla^2 V - \mathcal{L}(A^{-1}) \, A \right)^{-1} \, \nabla f \, d\mu .
\end{aligned}
$$

Generalized BL inequality and spectral gap

Theorem (Arnaudon, Bonnefont, J. ('18))

Let $x \in \mathbb{R}^n \to A(x) \in GL_n(\mathbb{R})$ be a smooth mapping such that $\nabla^2 V - \mathcal{L}(A^{-1})\, A$ is a symmetric positive definite matrix. Then,

$$\mathrm{Var}_\mu(f) \leq \int_{\mathbb{R}^n} \nabla f \cdot \left(\nabla^2 V - \mathcal{L}(A^{-1})\, A\right)^{-1} \nabla f \, d\mu.$$

Corollary

As a consequence, for all such matrices A,

$$\lambda_1 \geq \inf_{x \in \mathbb{R}^n} \rho\left(\nabla^2 V - \mathcal{L}(A^{-1})\, A\right)(x),$$

where, if M stands for some symmetric matrix, $\rho(M)$ denotes its smallest eigenvalue.

Generalized BL inequality and spectral gap

Why such a form $\nabla^2 V - \mathcal{L}(A^{-1})\, A$?

Through the Bakry-Émery Γ_2-calculus, the generalized BL inequality is equivalent to its dual form

$$\int_{\mathbb{R}^n} (Lf)^2 \, d\mu \;\geq\; \int_{\mathbb{R}^n} \nabla f \cdot \left(\nabla^2 V - \mathcal{L}(A^{-1})\, A\right) \nabla f \, d\mu,$$

which is true since

$$\int_{\mathbb{R}^n} (Lf)^2 \, d\mu \;=\; \int_{\mathbb{R}^n} \nabla f \cdot \nabla(-L) f \, d\mu$$

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the inequality being a generalization of Barta's inequality at the level of gradients.

Generalized BL inequality and spectral gap

Question: Case of equality in the generalized BL inequality ?

Answer: If H is some diffeomorphism on $\mathbb{R}^n$, then choose the matrix $A = (Jac\, H^T)^{-1}$, so that

$$\nabla^2 V - \mathcal{L}(A^{-1})\, A = -Jac\, \mathcal{L}H^T\, (Jac\, H^T)^{-1},$$

and provided this matrix is symmetric positive definite, then the equality holds for $f = \mathcal{L}H \cdot c$, with $c \in \mathbb{R}^n$ some constant vector, generalizing the extremal functions in the classical BL inequality: if $H = id$, then $\mathcal{L}id = -\nabla V$.

Question: Case of equality for the spectral gap ?

Answer: It depends on the structure of the associated eigenspace...

Generalized BL inequality and spectral gap

Example: The term involving the matrix A allows to compensate the lack of strong convexity, as in the following model: a Lipschitz perturbation of a non-strongly log-concave product measure.

The potential is

$$V(x) = \sum_{k=1}^{n} \frac{|x_k|^\alpha}{\alpha} + \beta \sum_{k=1}^{n} |x_k - x_{k+1}|, \quad x \in \mathbb{R}^n,$$

with $1 < \alpha < 2$.

Proposition

For β small enough, there exists $\lambda > 0$ such that for all $n \geq 1$, the spectral gap satisfies $\lambda_1 \geq \lambda$.

It seems that our approach goes beyond the classical method of requiring uniform estimate for the one-dimensional conditional distributions (Helffer, Ledoux, Gentil-Roberto in the end '90), for which some strong convexity at infinity is often needed.

Other consequences of the intertwining approach

- Second-order generalized BL inequalities (Bonnefont, J. ('18)), in the spirit of Cordero-Fradelizi-Maurey ('04) about the so-called B-conjecture.

  A second-order BL inequality is: for all f such that $\mathrm{Cov}_\mu(f, id) = 0$,

$$\mathrm{Var}_\mu(f) \leq \int_{\mathbb{R}^n} \nabla f \cdot \left(\nabla^2 V + \lambda_1 I_n\right)^{-1} \nabla f \, d\mu.$$

- Comparison of spectra of the diffusion operator $-L$ and the Schrödinger-type operators $-\mathcal{L} + \nabla^2 V$ and $-\mathcal{L}_A + M_A$ acting on gradients (Bonnefont, J. ('19); such a comparison has been emphasized in the non-weighted case by Johnsen ('00)):

$$\sigma(-L)\backslash\{0\} = \sigma(-\mathcal{L} + \nabla^2 V \mid_\nabla) = \sigma(-\mathcal{L}_A + M_A \mid_{A\nabla}).$$

- Optimality in dimension 1 and higher eigenvalues estimates (Bonnefont, J. ('19)).

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Optimality in dimension 1

In dimension 1, can we get the equality in

$$\lambda_1 \geq \sup_a \inf_{x\in\mathbb{R}} \left(V'' - a\,L(1/a)\right)(x) \quad ?$$

Taking the weight of the form $a = 1/h'$, with some function $h' > 0$, then

$$V'' - a\,L(1/a) = \frac{(-Lh)'}{h'}.$$

If the spectral gap λ_1 is attained, then the associated eigenfunction g_1 is strictly monotone with g_1' non-vanishing, so that taking $h = g_1$ entails the desired equality, recovering Chen's famous variational formula ('97) obtained by coupling.

Question: Does the intertwining approach allow to go beyond the spectral gap ?

Answer: Yes.

Higher order eigenvalues

Assume for simplicity that $\sigma_{ess}(-L) = \emptyset$, i.e., $\sigma(-L) = \sigma_{disc}(-L)$. The eigenvalues $(\lambda_n)_{n\in\mathbb{N}}$, ordered according to the Courant-Fisher min-max theorem, form a sequence tending to infinity as $n \to \infty$.

We have

$$\begin{aligned} L_a f &= Lf + 2\,a\left(\frac{1}{a}\right)' f' \\ &= f'' - V'\,f' - \log(a^2)'\,f' \\ &= f'' - V_a'\,f', \end{aligned}$$

with $V_a = V + \log(a^2)$, the associated invariant measure μ_a having Lebesgue-density proportional to $e^{-V_a} = e^{-V}/a^2$.

Higher order eigenvalues

The restriction to gradients being useless in dimension 1, the previous comparison of spectra rewrites as follows: letting $a = a_1$, then for all $k \in \mathbb{N}$,

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where $M_{a_1} = V'' - a_1\, L(1/a_1)$, which is for $k = 0$ the spectral gap estimate provided by the generalized BL inequality.

In dimension 1, we can iterate the argument: let us see how it works for $k = 1$: the intertwining with some smooth positive weight a_2 (say) applied to L_{a_1} gives

$$a_2\,(L_{a_1} f)' = (L_{a_1 \times a_2} - M_{a_1}^{a_2})\,(a_2\, f'),$$

where

$$M_{a_1}^{a_2} = V_{a_1}'' - a_2\, L_{a_1}(1/a_2).$$

Higher order eigenvalues

Hence,

$$\lambda_2(-L) \quad \geq \quad \lambda_1(-L_{a_1}) + \inf \ M_{a_1}$$

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Theorem

In the case $\sigma_{ess}(-L) = \emptyset$, we have for all $k \geq 1$,

$$\lambda_k(-L) = \sup_{a_1,\ldots,a_k>0} \inf\ M_{a_1} + \inf\ M_{a_1}^{a_2} + \ldots + \inf\ M_{a_1\ldots a_{k-1}}^{a_k},$$

the equality being satisfied when choosing the a_i conveniently in terms of the eigenfunctions $g_1, \ldots, g_k$.

Higher order eigenvalues

Choosing the $a_i = 1$ in the strongly convex case, we recover:

Theorem (Milman ('18))

Assume that V is strongly convex, i.e. $\inf V'' \geq \rho > 0$. *Then for all $k \geq 1$,*

$$\lambda_k(-L) \geq \lambda_k(-L_{OU,\rho}) \quad (= \rho\, k),$$

where

$$L_{OU,\rho} f(x) = f''(x) - \rho\, x\, f'(x), \quad V_{OU,\rho}(x) = \rho\, |x|^2/2.$$

We also prove an estimate on the gap between consecutive eigenvalues:

Theorem

Under the same assumption, we have for all $k \geq 1$,

$$\lambda_k - \lambda_{k-1} \geq \rho.$$

Higher order eigenvalues

A non-strongly convex example: Subbotin distribution:

$$V(x) = \frac{|x|^\alpha}{\alpha}, \quad 1 < \alpha \leq 2.$$

Choosing the $a_i = e^{\varepsilon_i V}$ for some convenient constants ε_i, then we get for all $k \geq 1$,

$$\lambda_k \geq C_{\alpha,\varepsilon} k^{2-\frac{2}{\alpha}-\varepsilon},$$

in accordance with Weyl's law describing the asymptotic behaviour of eigenvalues:

$$\lambda_k \underset{k\to\infty}{\simeq} C_\alpha k^{2-\frac{2}{\alpha}}.$$

Some perspectives and open questions

- Structure of the eigenspace associated to λ_1 (Barthe-Klartag, forthcoming).
- Iteration of the intertwinings, to recover and extend Milman's theorem.
- The case of Riemannian manifolds.
- Relate our Barta inequality to the dimensional aspect in the Bakry-Emery curvature-dimension criterion.
- Understand the probabilistic representation of the operator $\mathcal{L}_A$.
- Study the gap between consecutive eigenvalues in the non-strongly convex case, at least in dimension 1.
- Explore the consequences of the intertwinings in terms of:
  - Other functional inequalities (for instance log-Sobolev);
  - Stability by measure-transformation;
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    Steiner, forthcoming ?

As predicted by Jim Morrison, this is the end...

THANK YOU
FOR YOUR ATTENTION