Dynamic Γ-calculus and spectral monotonicity under heat flow

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Outline

1. Γ-calculus and Poincaré inequalities
2. Dynamic Γ-calculus and the main result

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1. Γ-calculus and Poincaré inequalities
2. Dynamic Γ-calculus and the main result

The classical Poincaré inequality

Poincaré, 1890: for any bounded domain $\Omega \subset \mathbb{R}^n$ there exists a constant $C > 0$ such that for every nice f with $\int_\Omega f = 0$,

$$\int_\Omega f^2 \leq C \int_\Omega |\nabla f|^2. \tag{1}$$

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By spectral theory, the smallest constant $C = C_P(\Omega)$ for which (1) holds is $\frac{1}{\lambda_1(-\Delta)}$, where $\lambda_1(-\Delta)$ is the smallest nonzero eigenvalue of the (Neumann) Laplacian on $L^2(\Omega)$.

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In general, a probability measure μ on a manifold is said to satisfy a Poincaré inequality with constant C if X is a random vector distributed uniformly on Ω and f is any sufficiently nice function,

$$\int f^2\, d\mu - \left(\int f\, d\mu\right)^2 \le C \int |\nabla f|^2\, d\mu.$$

A general framework for proving functional inequalities

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Δ generates a semigroup $(P_t)_{t\geq 0}$ of contraction operators on $L^1(\Omega)$, which acts to dissipate the energy. The P_t satisfy the equation

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Generalizing this framework gives Γ-calculus.

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In the Bakry-Émery framework, the basic ingredients are a measure space (Ω, μ) and a semigroup of contraction operators $(P_t)_{t\geq 0}$ on $L^1(\mu)$, which are assumed to preserve μ (i.e., $(P_t)_*\mu = \mu$ for all t) and satisfy some other natural conditions.

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Commonly, P_t is the semigroup associated to the law of an Itô diffusion, in which case L is a second-order differential operator. This is a helpful example to keep in mind, though the formalism is more general.

The "squares of fields" Γ and Γ_2

Given the generator L, we define the *carré du champ* $\Gamma(f,g)$ as

$$\Gamma(f,g) = \frac{1}{2}\left(L(fg) - f(Lg) - (Lf)g\right).$$

If L is a second-order derivative, then $\Gamma(f,g)$ will be a product of first-order derivatives of f and g. We usually abbreviate $\Gamma(f,f)$ by $\Gamma(f)$.

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Again integrating by parts, we see that under reversibility, $\int \Gamma_2(f,g)\,d\mu = \int (Lf)(Lg)\,d\mu$.

Γ-calculus: examples

- (Ω, g) is a Riemannian manifold, $\mu = d\,\mathrm{vol}_g$, and $L = L_g$ is the Laplace-Beltrami operator; then $\Gamma(f) = g(\nabla f, \nabla f)$ and

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  Γ_2 is an absolute mess... (see Klartag-Kozma-Ralli-Tetali, 2016)

The curvature condition $CD(K, \infty)$

Definiton

We say that (Ω, μ, Γ) satisfies the *curvature condition* $CD(K, \infty)$ if

$$\Gamma_2(f) \geq K\Gamma(f)$$

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The "ideal" methodology for applying Γ-calculus is to show that one's setting of interest satisfies some $CD(K, N)$ condition, and then argue that $CD(K, N)$ implies one's desired inequality solely from the algebra of the P_t, L, Γ, and Γ_2 operators.

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$$\Gamma_2(f) = \|\nabla^2 f\|^2 + \mathrm{Ric}(rS^n)(\nabla f, \nabla f) \geq \frac{1}{r^2}|\nabla f|^2 = \frac{1}{r^2}\Gamma(f),$$

  i.e., rS^n satisfies $CD(\frac{1}{r^2},\infty)$.

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  i.e., rS^n satisfies $CD(\frac{1}{r^2},\infty)$.
- If $\Omega = (\mathbb{R}^n, \mu, L_\mu)$ where $d\mu = e^{-W}\,dx$ is log-concave,

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  If $\nabla^2 W \geq K I_n$ (e.g., the Gaussian), then Ω satisfies $CD(K, \infty)$.

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    - Also integrated forms of these inequalities: hypercontractivity, exponential decay of entropy, reverse Hölder inequality for eigenvectors...
- Equivalence (up to universal constants) of isoperimetry, spectral gap, and exponential concentration under $CD(0,\infty)$ (Ledoux 2004, E. Milman 2009).
- Stochastic localization: bound the isoperimetric constant of an isotropic log-concave measure by decomposing it into $CD(K,\infty)$-pieces (Eldan 2015, Lee-Vempala 2017, Chen 2021)

An example functional inequality: $CD(K,\infty) \Rightarrow \mathrm{Poin}(\frac{1}{K})$

Theorem

Suppose (Ω, μ, Γ) satisfies the curvature condition $CD(K,\infty)$. Then Ω satisfies a Poincaré inequality with constant $\frac{1}{K}$.

An example functional inequality: $CD(K,\infty) \Rightarrow \mathrm{Poin}(\frac{1}{K})$

Main lemma

For $0 < s < t$,

$$\frac{d}{ds} P_{t-s}(P_s(f)^2) = -P_{t-s}(\Gamma(P_s(f))) \tag{2}$$

$$\frac{d}{ds} P_{t-s}(\Gamma(P_s(f))) = -P_{t-s}(\Gamma_2(P_s(f))) \tag{3}$$

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The proof of the lemma follows directly from $\frac{d}{ds}P_s = LP_s = P_sL$ and the definitions of Γ, Γ_2.

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Integrating (2) over time, we get $P_t(f^2) - P_t(f)^2 = \int_0^t P_{t-s}(\Gamma(P_s(f)))$.

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Integrating (2) over time, we get $P_t(f^2) - P_t(f)^2 = \int_0^t P_{t-s}(\Gamma(P_s(f)))$. Integrating over $d\mu$, sending t to ∞, and using $\int P_s(\cdot)\, d\mu = \int (\cdot)\, d\mu$, $\lim_{t\to\infty} P_t(f) = \int f\, d\mu$ gives

Corollary 1

$$\int f^2\, d\mu - \left(\int f\, d\mu\right)^2 = \int_0^\infty dt \int_\Omega \Gamma(P_t(f))\, d\mu \quad (4)$$

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Let $\Lambda(s) = P_{t-s}(\Gamma(P_s(f)))$; then by (3) and the assumption of $CD(K,\infty)$, $\Lambda'(s) \leq -K\Lambda(s)$, i.e., $\Lambda(t) \leq e^{-Kt}\Lambda(0)$, yielding

Corollary 2

$$\Gamma(P_t(f)) \leq e^{-Kt} P_t(\Gamma(f))$$

$CD(K,\infty) \Rightarrow \mathrm{Poin}(\frac{1}{K})$, continued

We have seen:

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Combining these two and again using $\int P_t(\cdot)\,d\mu = \int (\cdot)\,d\mu$, we obtain

$$\int f^2\,d\mu - \left(\int f\,d\mu\right)^2 \le \int_0^\infty \left(e^{-Kt}\int_\Omega \Gamma(f)\,d\mu\right) = \frac{1}{K}\int_\Omega \Gamma(f)\,d\mu$$

which is what we wanted.

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2. Dynamic Γ-calculus and the main result

The adjoint to the heat semigroup

Let ρ be a probability density on $\mathbb{R}^n$, and let $(P_t)_{t\geq 0}$ be the usual heat semigroup; we scale time so that the generator is $\frac{\Delta}{2}$. Define

$$\rho_t := P_t(\rho) = \rho * \gamma_t,$$

where $\gamma_t(x) = (2\pi t)^{-n/2} e^{-|x|^2/2t}$ is the density of the standard Gaussian of covariance $\sqrt{t} I_n$. ρ_t satisfies the classical heat equation $\partial_t \rho_t = \frac{\Delta}{2} \rho_t$.

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Remark

Prékopa-Leindler: if ρ is log-concave then so is ρ_t.

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$$\int Q_t(f) g \cdot \rho_t = \int f P_t(g) \cdot \rho = \int P_t(f\rho) g \Rightarrow Q_t(f) = \frac{P_t(\rho f)}{P_t(\rho)}$$

The "infinitesimal generator" $\Box_t$

Definiton

$Q_t : L^2(\rho) \to L^2(\rho_t) \qquad Q_t(f) = \frac{P_t(\rho f)}{P_t(\rho)}$

Using the heat equation $\partial_t P_t = \frac{\Delta}{2} P_t$, one computes explicitly that $\partial_t Q_t(f) = \frac{1}{2}\Box_t Q_t(f)$, where

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$$\Box_t = \Delta + 2(\nabla \log \rho_t) \cdot \nabla.$$

The "box operator" is similar to the Laplace operator $L_t := L_{\rho_t}$ defined above, which generates the semigroup with invariant measure ρ_t, but it's not quite the same: in fact, we have

$$\Box_t = L_t + (\nabla \log \rho_t) \cdot \nabla.$$

The "infinitesimal generator" $\Box_t$, continued

Note that $(Q_t)_{t\geq 0}$ isn't a semigroup; for $t \neq s$, Q_t and Q_s don't even operate on the same Hilbert space.

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$$Q_{t,s}(f) = \frac{P_{t-s}(\rho_s f)}{P_{t-s}(\rho_s)},$$

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This gives the "inhomogeneous semigroup equation"

$$Q_{u,t} \circ Q_{t,s} = Q_{u,s}$$

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For $f \in L^2(\rho_s)$, we get $\partial_t Q_{t,s}(f) = \Box_t Q_{t,s} f$, as before, and also $\partial_s Q_{t,s}(f) = -Q_{t,s}(\Box_s f)$.

Γ-calculus for Q_t

Fix $t \geq 0$. We can define Γ and Γ_2 for $\Box_t$ just as for L_t; one computes explicitly that $\Gamma^{\Box_t}(f) = |\nabla f|^2 = \Gamma^{L_t}(f)$, while

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Recall the computation for the usual Markov semigroup P_t:

Main lemma

For $0 < s < t$,

$$\frac{d}{ds} P_{t-s}(P_s(f)^2) = -P_{t-s}(\Gamma(P_s(f))) \tag{4}$$

$$\frac{d}{ds} P_{t-s}(\Gamma(P_s(f))) = -P_{t-s}(\Gamma_2(P_s(f))) \tag{5}$$

Γ-calculus for Q_t

Fix $t \geq 0$. We can define Γ and Γ_2 for $\square_t$ just as for L_t; one computes explicitly that $\Gamma^{\square_t}(f) = |\nabla f|^2 = \Gamma^{L_t}(f)$, while

$$\Gamma_2^{\square_t}(f) = \|\nabla^2 f\|^2 - 2\langle(\nabla^2 \log \rho_t)\nabla f, \nabla f\rangle = \Gamma_2^{L_t}(f) - \langle(\nabla^2 \log \rho_t)\nabla f, \nabla f\rangle.$$

For Q_t, the same computation gives essentially the same formulas:

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For $0 < s < t$,

$$\frac{d}{ds} Q_{t,s}(Q_s(f)^2) = -Q_{t,s}(\Gamma(Q_s(f))) \tag{4}$$

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Application: spectral monotonicity

Theorem (Klartag-P., 2021)

Let ρ be a log-concave density on $\mathbb{R}^n$, $\rho_t = \rho * \gamma_t$. Then $C_P(\rho_t)$ is an increasing function of t.

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Let ρ be a log-concave density on $\mathbb{R}^n$, $\rho_t = \rho * \gamma_t$. Then $C_P(\rho_t)$ is an increasing function of t.

We have $C_P(\rho_t)^{-1} = \inf_{\varphi \perp 1} \frac{\int |\nabla \varphi|^2 \rho_t}{\int f^2 \rho_t} = \inf_{\varphi \perp 1} R_t(\varphi)$, where

$$R_t(\varphi) = \frac{\int \Gamma(\varphi)\, \rho_t}{\int \varphi^2 \rho_t}$$

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Claim

The "Rayleigh quotient decreases along the heat flow": that is, for any $\varphi \perp 1 \in L^2(\rho)$, $R_t(\varphi_t)$ is decreasing, where $\varphi_t = Q_t(\varphi)$.

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By the definition of $C_P(\rho_t)^{-1}$ as an infimum, this clearly implies that $C_P(\rho_t)^{-1}$ is nondecreasing, and so $C_P(\rho_t)$ is nonincreasing.

Monotonicity of the Rayleigh quotient (1)

Main lemma

For $0 < s < t$,

$$\frac{d}{ds} Q_{t,s}(\varphi_s^2) = -Q_{t,s}(\Gamma(\varphi_s))$$
$$\frac{d}{ds} Q_{t,s}(\Gamma(\varphi_s)) = -Q_{t,s}(\Gamma_2^{\square_s}(\varphi_s))$$

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If we integrate both sides against ρ_t and use $\int Q_{t,s}(f)\rho_t = \int f\, \rho_s$, we can throw out the $Q_{t,s}$ and obtain

Main lemma, integrated

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$$\frac{d}{ds} \int \varphi_s^2\, \rho_s = -\int \Gamma(\varphi_s)\, \rho_s$$
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For $0 < s < t$,

$$\frac{d}{ds}\|\varphi_s\|^2_{L^2(\rho_s)} = -\int \Gamma(\varphi_s)\,\rho_s,$$
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Applying this immediately yields

$$\frac{d}{ds}R_s(\varphi_s) = \frac{\left(\int \Gamma(\varphi_s)\,\rho_s\right)^2 - \|\varphi_s\|_{L^2(\rho_s)}\int \Gamma_2^{\Box_t}(\varphi_s))\,\rho_s}{\|\varphi_s\|^4_{L^2(\rho_s)}}.$$

We need to show that the numerator is always negative.

Monotonicity of the Rayleigh quotient (3)

To show:

$$\left(\int \Gamma(\varphi_s)\,\rho_s\right)^2 - \|\varphi_s\|_{L^2(\rho_s)} \int \Gamma_2^{\square_s}(\varphi_s))\,\rho_s \leq 0. \tag{6}$$

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$$\left(\int \Gamma(\varphi_s)\,\rho_s\right)^2 - \|\varphi_s\|_{L^2(\rho_s)} \int \Gamma_2^{\Box_s}(\varphi_s))\,\rho_s \le 0. \tag{6}$$

Recall our integration by parts formulas ($L_s = L_{\rho_s}$, as before):

$$\int \Gamma(\varphi_s)\,\rho_s = \int \varphi_s \cdot (-L_s\varphi_s)\,\rho_s, \qquad \int \Gamma_2^{L_s}(\varphi_s)\,\rho_s = \int (-L_s\varphi_s)^2\,\rho_s.$$

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By Cauchy-Schwarz, we thus immediately obtain

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This is almost, but not quite, the LHS of (6).But recall that

$$\Gamma_2^{\Box_s}(\varphi_s)) = \Gamma_2^{L_s}(\varphi_s)) - \langle(\nabla^2 \log \rho_s)\varphi_s, \varphi_s\rangle,$$

and log-concavity of ρ_s implies that the second term is positive. Hence the LHS of (6) is negative, and we are done.

Remarks (1)

Note that our argument does not assume that the Poincaré constant of ρ is attained by some function f (which would then be a Neumann eigenfunction), which is important because this assumption is not always satisfied in practice: in fact, $C_P(\nu)$ is not attained when ν is the exponential distribution.

Remarks (1)

As it turns out, if $\rho = e^{-W}$ is log-concave and W is *supercoercive* – $\frac{W(x)}{|x|} \to \infty$ as $x \to \infty$ – then L_ρ has a discrete spectrum. In this case, the monotonic decrease of the Rayleigh quotient along the heat flow, along with the min-max characterization of eigenvalues, suggests that the entire spectrum of L_{ρ_s} should *strictly* decrease with s.

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We can in fact show this under an additional technical assumption on the decay of the eigenfunctions, which is known to be satisfied if a slightly stronger growth condition on W holds:

Theorem (Klartag-P., 2021)

Let $\rho = e^{-W}$ be a log-concave measure, and suppose that $\frac{|\nabla W|^2}{4} - \frac{\Delta W}{2} \to \infty$ as $x \to \infty$. Then the spectrum of ρ_s is monotonically strictly decreasing with s.

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We do not know if the assumption on W can be removed.

Remarks (2)

After developing the dynamic Γ-calculus approach, we found a totally different (and simpler) approach which actually yields stronger results. Following ideas of Kim and Milman, we were able to construct a family of maps $T_s : \mathbb{R}^n \to \mathbb{R}^n$ such that T_s pushes ρ_s forward onto ρ, and T_s is a contraction, i.e., a 1-Lipschitz map.

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The argument that if T is a contraction pushing μ onto ν then $C_P(\nu) \leq C_P(\mu)$ is a single line: for any $f \in L^2(\nu)$, $f \perp 1$,

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By essentially the same argument, the existence of a family of contractions yields monotonicity not only of the Poincaré constant and of the entire spectrum (when it exists), but of the log-Sobolev constant (if finite) and constants in other functional inequalities.

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Thank you!