Ricci curvature of Markov chains via convexity of the entropy

Jan Maas
University of Bonn

6ICSA Bedlewo
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Joint work with Matthias Erbar (Bonn)

Starting point: Displacement convexity of the entropy

Connection between:

- Boltzmann-Shannon entropy:

$$\mathrm{Ent}(\mu) = \int_{\mathbf{R}^n} \rho(x) \log \rho(x) \, \mathsf{d}x; \qquad \frac{d\mu}{dx} = \rho$$

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- L^2-Wasserstein metric:

$$W_2(\mu_0, \mu_1)^2 = \inf \left\{ \int_{\mathbf{R}^n \times \mathbf{R}^n} |x - y|^2 \, \mathsf{d}\gamma(x, y) \right. \\ \left. : \gamma \text{ with marginals } \mu_0 \text{ and } \mu_1 \right\}$$

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Theorem (McCann '94)

The Boltzmann-Shannon entropy is convex along geodesics in $(\mathcal{P}(\mathbf{R}^n), W_2)$.

Starting Point: Ricci curvature and optimal transport

Theorem (Otto, Villani; Cordero-Erausquin, McCann, Schmuckenschläger; von Renesse, Sturm)

For a Riemannian manifold $\mathcal{M}$, TFAE:

1. $\mathrm{Ric} \geq \kappa$ everywhere on $\mathcal{M}$
2. Displacement κ-convexity of the entropy, i.e.,

$$\mathrm{Ent}(\mu_t) \leq (1-t)\mathrm{Ent}(\mu_0) + t\mathrm{Ent}(\mu_1) - \frac{\kappa}{2} t(1-t) W_2^2(\mu_0, \mu_1)$$

   for all L^2-Wasserstein geodesics $(\mu_t)_{t\in[0,1]}$ in $\mathcal{P}(\mathcal{M})$.

Synthetic Ricci curvature of metric measure spaces

Definition (Lott, Villani; Sturm)

A metric measure space $(\mathcal{X}, d, m)$ satisfies $CD(\kappa, \infty)$ if any $\mu_0, \mu_1 \in \mathcal{P}_2(\mathcal{X})$ can be connected by a constant speed W_2-geodesic $(\mu_t)_{t\in[0,1]}$ such that

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But..... what about discrete spaces?

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$\longrightarrow$ $(\alpha(t))$ is 2-Hölder, hence constant.

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LSV-definition does not apply to discrete spaces.

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How to make sense of gradient flows in metric spaces?

Let $\varphi : \mathbf{R}^n \to \mathbf{R}$ smooth and convex. For $u : \mathbf{R}_+ \to \mathbf{R}^n$ TFAE:

1. u solves the gradient flow equation $u'(t) = -\nabla\varphi(u(t))$.
2. u solves the evolution variational inequality

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|u(t) - y|^2 \leq \varphi(y) - \varphi(u(t)) \qquad \forall y .$$

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The heat flow is the gradient flow of the entropy w.r.t W_2 , i.e.,

$$\partial_t \mu = \Delta \mu \quad \iff \quad \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t} W_2(\mu_t, \nu)^2 \leq \mathrm{Ent}(\nu) - \mathrm{Ent}(\mu_t) \qquad \forall \nu$$

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Many extensions have been proved:

• $\mathbf{R}^n$	Jordan–Kinderlehrer–Otto
• Riemannian manifolds	Villani, Erbar
• Hilbert spaces	Ambrosio–Savaré–Zambotti
• Finsler spaces	Ohta–Sturm
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Question

Is there a version of the JKO-Theorem for *discrete* spaces?

Discrete setting

Setting

- $\mathcal{X}$: finite set
- $K : \mathcal{X} \times \mathcal{X} \to \mathbf{R}_+$ Markov kernel, i.e., $\forall x \;:\; \sum_y K(x,y) = 1$

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- K is irreducible $\longrightarrow$ $\exists!$ inv. measure π
- π is reversible i.e., $\forall x, y \; : \; K(x,y)\pi(x) = K(y,x)\pi(y)$

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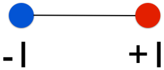
Relative Entropy

- For $\rho \in \mathcal{P}(\mathcal{X}) := \left\{ \rho : \mathcal{X} \to \mathbf{R}_+ \ \middle| \ \sum_{x \in \mathcal{X}} \rho(x)\pi(x) = 1 \right\}$,

$$\mathrm{Ent}(\rho) = \sum_{x \in \mathcal{X}} \rho(x) \log \rho(x) \, \pi(x) \, .$$

Simplest non-trivial example: 2-point space

$\mathcal{X} = \{-1, 1\}$
$K(-1, 1) = K(1, -1) = 1$
$\pi(-1) = \pi(1) = \frac{1}{2}$



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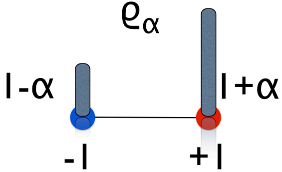

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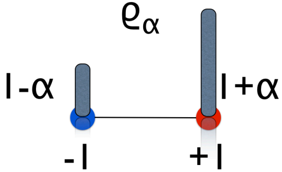

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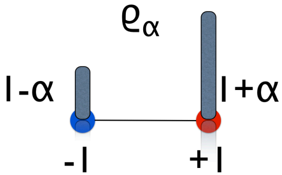

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Answer

NO! Reason:
$W_2(\rho_\alpha, \rho_\beta) = \sqrt{2|\beta - \alpha|}$.

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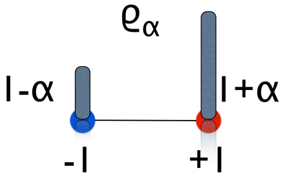

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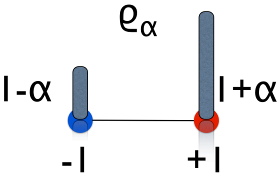

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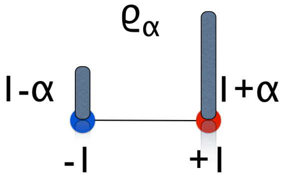

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Proposition [M. 2011]

The heat flow is the gradient flow of Ent w.r.t. the metric $\mathcal{W}$, where

$$\mathcal{W}(\rho_\alpha, \rho_\beta) := \frac{1}{\sqrt{2}} \int_\alpha^\beta \sqrt{\frac{\operatorname{arctanh} r}{r}}\, \mathrm{d}r, \qquad -1 \leq \alpha \leq \beta \leq 1.$$

How to define $\mathcal{W}$ in the general discrete case?

In $\mathbf{R}^n$ there is a dynamical characterisation of W_2:

Benamou-Brenier formula in $\mathbf{R}^n$

$$W_2(\bar{\rho}_0, \bar{\rho}_1)^2 = \inf_{\rho_\cdot, \Psi_\cdot} \left\{ \int_0^1 \int_{\mathbf{R}^n} |\Psi_t(x)|^2 \, \rho_t(x) \, \mathrm{d}x \, \mathrm{d}t \;\; : \right.$$
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- Obstruction: how to multiply probability densities and discrete gradients?

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How should we define $\hat\rho$? $\longrightarrow$ logarithmic mean

$$\hat\rho(x,y) := \int_0^1 \rho(x)^{1-\alpha}\rho(y)^{\alpha}\,\mathrm{d}\alpha = \frac{\rho(x)-\rho(y)}{\log\rho(x)-\log\rho(y)}$$

Results

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Remark

Related independent work by

- Chow, Huang, Li, and Zhou
- Mielke

Why the logarithmic mean?

Formal proof of the JKO-Theorem

1. If (ρ_t, ψ_t) satisfy the cont. eq. $\partial_t \rho + \nabla \cdot (\rho \nabla \psi) = 0$, then

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ent}(\rho_t) = -\langle \log \rho_t, \nabla \cdot (\rho_t \nabla \psi_t) \rangle = \langle \nabla \log \rho_t, \nabla \psi_t \rangle_{\rho_t} \; .$$

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2. If ρ_t solves the heat equation in $\mathbf{R}^n$, then

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Logarithmic mean compensates for the lack of a discrete chain rule:

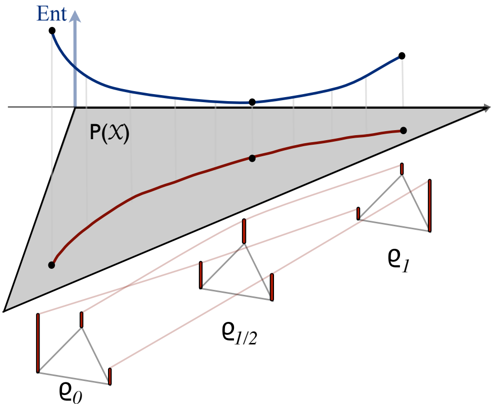
$$\rho(x) - \rho(y) = \hat{\rho}(x,y)\big(\log \rho(x) - \log \rho(y)\big)$$

Ricci curvature of Markov chains

The discrete analogue of Lott–Sturm–Villani becomes:

Definition (Erbar, M. 2011)

We say that $(\mathcal{X}, K, \pi)$ has Ricci curvature bounded from below by $\kappa \in \mathbf{R}$ if the entropy is κ-convex along geodesics in $(\mathcal{P}(\mathcal{X}), \mathcal{W})$.



Consequences: Sharp functional inequalities

Theorem (Erbar, M.)

Let $(\mathcal{X}, K, \pi)$ be a reversible Markov chain. Let $\kappa > 0$.

1. à la Bakry–Émery: $\mathrm{Ric}(K) \geq \kappa \Longrightarrow$ modified log-Sobolev, i.e.

$$\mathrm{Ent}(\rho) \leq \frac{1}{2\kappa}\mathcal{E}(\rho, \log \rho)\ .$$

   This implies $\mathrm{Ent}(H_t\rho) \leq e^{-2\kappa t}\,\mathrm{Ent}(\rho)$.

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3. mod. Talagrand $\Longrightarrow$ [spectral gap and T_1]:

$$\|\varphi\|^2_{L^2(\mathcal{X},\pi)} \leq \frac{1}{\kappa}\mathcal{E}(\varphi, \varphi) \quad \text{and} \quad W_1(\rho, \mathbf{1})^2 \leq \frac{1}{\kappa}\,\mathrm{Ent}(\rho)\ .$$

Ricci bounds: examples

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Theorem (Erbar, M. 2012)

Let $(\mathcal{X}_i, K_i, \pi_i)$ be reversible finite Markov chains and let $(\mathcal{X}, K, \pi)$ be the product chain. Then:

$$\mathrm{Ric}(\mathcal{X}_i, K_i, \pi_i) \geq \kappa_i \qquad \Longrightarrow \qquad \mathrm{Ric}(\mathcal{X}, K, \pi) \geq \frac{1}{n} \min_i \kappa_i$$

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- Dimension-independent bounds
- Sharp bounds for the discrete hypercube $\{-1, 1\}^n$

Gromov-Hausdorff convergence

- Let $\mathbf{T}_N^d = (\mathbf{Z}/N\mathbf{Z})^d$ be the discrete torus.
- Let $\mathcal{W}_N$ be the renormalised transportation metric for simple random walk on $\mathbf{T}_N^d$.

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- Compatibility between W_2 and $\mathcal{W}$.
- Main ingredient for proving convergence of gradient flows.

Further developments

- Systems of reaction-diffusion equations (Mielke)
- Fractional heat equations (Erbar)
- Dissipative quantum mechanics (Carlen, M.; Mielke)

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Thank you!