Ricci curvature of finite Markov chains via convexity of the entropy

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Overview

What we are talking about

RICCI CURVATURE

OPTIMAL TRANSPORT

- Wasserstein geometry
- Convexity of Shannon's entropy

MARKOV CHAINS

General theoretical framework

The heat flow is the gradient flow of the entropy in the W_2 space

$\mathrm{Ric} \geq \kappa \iff \kappa$-convexity of the entropy $\iff \kappa$-contractivity of the heat flow

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Interpret the continuous time Markov chain as the heat flow (via semigroup)

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$\star$ Define a geometry $\mathcal{W}$ such that heat flow with a Markov kernel is the gradient flow of entropy $\star$

Why do we care?

Mainly three motivations:

- obtain convergence to equilibrium of Markov chains
- study the geometry induced by Markov kernel (e.g. random walk on the hypercube, graphs)
- obtain discrete counterpart of powerful inequalities (e.g. mass concentration, Sobolev inequalities, spectral results)

History on Ricci curvature and evolution of the heat flow

- McCann [1997] (displacement convexity on $\mathbb{R}^n$)
- Jordan-Kinderlehrer-Otto seminal work [1998]

- Otto–Villani [2000] (extension to manifold, Hessian of entropy on $\mathscr{P}(M)$)

- Cordero–Erausquin, McCann, Schmuckenschläger & von Renesse–Sturm [2005] (rigorous result on convexity and Ricci)

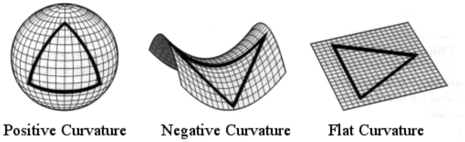
- Lott–Villani [2009] & Sturm [2006] (Ricci for metric measure spaces)

- Maas [2011] & Erbar–Maas [2012] among others (Ricci for discrete spaces)

Ricci Curvature

Ricci curvature governs how volumes are distorted on the space

$\mathrm{Ric}_{\mathbb{R}^n} \equiv 0$



Why a lower bound? $\quad (X, Y) \to \mathrm{Ric}(X, Y) \in \mathbb{R}$

- Analytical results (functional inequalities)
- Contraction properties
- Topological obstruction

Optimal transport I

Metric space $(\mathcal{X}, d)$

Space of probability measures
$\mathscr{P}(\mathcal{X}) = \{\mu : X \to \mathbb{R}_+ : \mu$ additive, $\mu(\mathcal{X}) = 1\}$

- The optimal transport problem:

$$\inf_{\gamma} \left\{ \int_{X \times X} c(x,y) \ \mathrm{d}\gamma(x,y) : \gamma \in \Gamma(\mu_0, \mu_1) \right\} \qquad \text{(K)}$$

  for $\mu_0, \mu_1 \in \mathscr{P}(\mathcal{X})$,
- Endow $\mathscr{P}(\mathcal{X})$ with the *2-Wasserstein distance* W_2:

$$W_2^2(\mu_0, \mu_1) := \min_{\gamma} \left\{ \int_{X \times X} d^2(x,y) \ \mathrm{d}\gamma(x,y) : \gamma \in \Gamma(\mu_0, \mu_1) \right\}$$

Optimal transport II

- Dynamic formulation relevant for us (Benamou-Brenier):
  Given b vector field and μ measure,

  $$\mathcal{A}(b, \mu) := \int_{\mathcal{X}} |b|^2 \, \mathrm{d}\mu$$

  Take μ_t curve on the space of measures
  $\mu : [0, 1] \to \mathscr{P}(\mathcal{X}), t \mapsto \mu_t$ from μ_0 to μ_1

  $$W_2^2(\mu_0, \mu_1) = \min_{b,\mu} \left\{ \int_0^1 \mathcal{A}(b_t, \mu_t) \, \mathrm{d}t : \frac{\mathrm{d}}{\mathrm{d}t}\mu_t + \mathrm{div}(b_t \mu_t) = 0 \right\}$$

  The minimizer is a geodesic.

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Optimal transport provides the space of probability measures a geometry in the space of probability measures

Optimal transport III

We consider a reference measure $\pi \in \mathscr{P}(\mathcal{X})$ and absolutely continuous measures $\mu = \rho\pi$, ρ density

- W convexity of the entropy:

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

- Gradient flow (high-level!): given a function f with $Dom(f) \subset \mathcal{X}$, $x_t : I \to Dom(f)$ is a gradient flow for f if

$$x_t' = -\nabla f(x_t)$$

Heat flow

Consider heat propagating on a space $\mathcal{X}$ and a temperature function $u(x,t)$ for $x \in \mathcal{X}$ and $t \in [0,T]$,
the heat equation is

$$\frac{\mathrm{d}}{\mathrm{d}t}u(t) = \operatorname{div} \nabla u = \Delta u$$

Heat semigroup $P_t := e^{t\Delta}$

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$\star$ Interpret our continuous time Markov chain as the heat flow $\star$

Our setting

Finite space of states $\mathcal{X}$, irreducible, reversible Markov kernel K

$$K(x_i, x_j) \; = \; K_{ij} \; = \; \Pr\big(X_t = x_j \mid X_{t-1} = x_i\big), \quad \sum_j K(x_i, x_j) = 1$$

Unique steady state $\quad \pi = \pi K$

Continuous time Markov semigroup

$P_t := e^{t(K-I)}$ Markov generator

$$\Delta := \operatorname{div} \nabla = K - I$$

Space of probability densities

$$\mathscr{P}(\mathcal{X}) := \Big\{ \rho : \mathcal{X} \to \mathbb{R}_+ : \sum_{x \in \mathcal{X}} \rho(x)\, \pi(x) = 1 \Big\}$$

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$\star$ We would like to study the geometry induced by K $\star$

New distance $\mathcal{W}$

Discrete action:

$$\mathcal{A}(\psi,\rho) := \frac{1}{2}\sum_{x,y\in\mathcal{X}} (\psi(y)-\psi(x))^2\hat{\rho}(x,y)K(x,y)\pi(x) = ||\nabla\psi||_\rho^2$$

Definition

For $\rho_0, \rho_1 \in \mathscr{P}(\mathcal{X})$ we define

$$\mathcal{W}^2(\rho_0,\rho_1) := \inf_{\psi,\rho}\left\{ \int_0^1 \mathcal{A}(\psi_t,\rho_t)\,\mathrm{d}t : \frac{\mathrm{d}}{\mathrm{d}t}\rho_t + \mathrm{div}(\hat{\rho}_t\nabla\psi_t) = 0\right\}$$

with ρ_t, ψ_t sufficiently regular.

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Theorem

The heat flow $\rho_t := P_t\rho$ is the gradient flow of Shannon's entropy $\mathcal{H}(\rho) = \sum_x \rho\log\rho\pi$

$$\mathsf{grad}_{\mathcal{W}}\mathcal{H}(\rho_t) = \nabla\log(\rho_t) = -\nabla\psi_t$$

Defining Ricci

Definition

We say that K has a Ricci curvature bounded by below by $\kappa \in \mathbb{R}$ if for any geodesic $\{\rho_t\}_{t\in[0,1]}$ in $(\mathscr{P}(\mathcal{X}), \mathcal{W})$ we have

$$\mathcal{H}(\rho_t) \leq (1-t)\mathcal{H}(\rho_0) + t\mathcal{H}(\rho_1) - \frac{\kappa}{2}t(1-t)\mathcal{W}^2(\rho_0, \rho_1)$$

and we write

$$\mathrm{Ric}_K \geq \kappa$$

Equivalent notions to Ricci

Theorem

Let $\kappa \in \mathbb{R}$. For an irreducible and reversible Markov kernel $(\mathcal{X}, K)$ TFAE:

(i) $\mathrm{Ric}_K \geq \kappa$;

(ii) For all $\rho_0, \rho_1 \in \mathscr{P}(\mathcal{X})$ the following 'evolution variational inequality' holds for all $t \geq 0$:

$$\frac{1}{2}\frac{\mathrm{d}^+}{\mathrm{d}t}\mathcal{W}^2\big(P_t\rho_0, \rho_1\big) + \frac{\kappa}{2}\mathcal{W}^2\big(P_t\rho_0, \rho_1\big) \leq \mathcal{H}(\rho_1) - \mathcal{H}\big(P_t\rho_0\big);$$

(iii) For all $\rho \in \mathscr{P}(\mathcal{X})$

$$\mathrm{Hess}\, \mathcal{H}(\rho) \geq \kappa;$$

(iv) For all $\rho_0, \rho_1 \in \mathscr{P}(\mathcal{X})$, there exists a constant speed geodesic $(\rho_t)_{t \in [0,T]}$ that connects them along which Shannon's entropy is κ-convex

κ-contractivity

Proposition

Let $(\mathcal{X}, K)$ be as before, with $\mathrm{Ric}_K \geq \kappa$. Then the continuous time Markov semigroup $(P_t)_{t\geq 0}$ satisfies

$$\mathcal{W}(P_t\rho_0, P_t\rho_1) \leq e^{-\kappa t}\mathcal{W}(\rho_0, \rho_1)$$

for all $\rho_0, \rho_1 \in \mathscr{P}(\mathcal{X})$ and $t \geq 0$.

Tensorisation result

Stability of our definition of Ricci for operations on the Markov chain

$\mathcal{X} = \prod_{i=1}^{n} \mathcal{X}_i\,,\ \ \sum_{i=1}^{n} \alpha_i = 1\,,\ \ X = (X_1, \ldots, X_n)\,,$ Kernel of the product chain on $\mathcal{X}$ is K_α

$$K_\alpha(x,y) = \begin{cases} \sum_i \alpha_i K_i(x_i, x_i), & x_i = x_i \,\forall i \\ \alpha_i K_i(x_i, y_i) & x_i \neq y_i \text{ and } x_j = y_j \,\forall i \neq j \\ 0 & \text{otherwise} \end{cases}$$

Theorem

Assume that $\mathrm{Ric}_{K_i} \geq \kappa_i$ for $i = 1, \ldots, n$. Then we have

$$\mathrm{Ric}_{K_\alpha} \geq \min_i \alpha_i \kappa_i$$

Ricci of a random walk on the discrete hypercube

Let $\mathcal{Q} = \{0,1\}$, $(\mathcal{Q}, K_{p,q})$, $\quad K(0,1) = p, K(1,0) = q$ for $p, q \in (0,1)$

Any measure $\mu \in \mathscr{P}(\mathcal{Q})$ is $\mu = (1-\lambda)\delta_0 + \lambda\delta_1$ for $\lambda \in [0,1]$

Steady state is π with $\lambda = \frac{p}{p+q}$

Let us look at $(\mathcal{Q}^n, K_p)$ simple random walk on n-dimensional hypercube, with $\alpha_i = 1/n$. Maas proves

$$\mathrm{Ric}_{K_p} \geq \kappa_p := p + p \cdot \frac{1}{2} \inf_{\lambda} \left\{ \frac{1}{\lambda(1-\lambda)} \cdot \theta(\lambda, 1-\lambda) \right\}$$

Then by tensorisation

$$\mathrm{Ric}_{K_{p,n}} \geq \frac{1}{n} 2p$$

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Thank you!

Extra: Functional inequalities

Theorem

Let K be an irreducible and reversible Markov kernel on a finite set $\mathcal{X}$ with $\mathrm{Ric}_K \geq \kappa$ or $\mathrm{Ric} \geq \lambda > 0$. The following inequalities hold:

$$\mathcal{H}(\rho) \;\leq\; \mathcal{W}(\rho, \mathbf{1})\sqrt{\mathcal{I}(\rho)} - \frac{\kappa}{2}\mathcal{W}(\rho, \mathbf{1})^2 \qquad (\mathrm{HWI}(\kappa))$$

$$\mathcal{H}(\rho) \;\leq\; \frac{1}{2\lambda}\mathcal{I}(\rho) \qquad (\mathrm{MLSI}(\lambda))$$

$$\mathcal{W}(\rho, \mathbf{1}) \;\leq\; \sqrt{\frac{2}{\lambda}\mathcal{H}(\rho)} \qquad (\mathrm{T}_{\mathcal{W}}(\lambda))$$

$$||\varphi||_\pi^2 \;\leq\; \frac{1}{\lambda}||\nabla\varphi||_\pi^2 \qquad (\mathrm{P}(\lambda))$$

holds for all functions $\psi : \mathcal{X} \to \mathbb{R}$.