

Poincaré, modified logarithmic Sobolev and isoperimetric inequalities for Markov chains with non-negative Ricci curvature

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Poincaré, modified logarithmic Sobolev and isoperimetric inequalities for Markov chains with non-negative Ricci curvature
as a follow up of
Ricci curvature of finite markov chains via convexity of the entropy

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1. The main goal (of the first paper) is to introduce a new geometric structure in the study of Markov semigroups (Markov chains)
2. This is done via an interpretation of the semigroup as a gradient flow of the Shannon entropy
3. Leading to a synthetic notion of Ricci curvature to study contraction properties

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New ingredients (content of the new paper): functional inequalities and applications to bounds on the mixing time of the chain and to its convergence to equilibrium

Road from old paper to present

- ▶ Geometric structure on space of Markov chains
- ▶ Synthetic notion of Ricci curvature ($\text{Ric} \geq 0$)
- ▶ Analogous version of functional inequalities for Markov chains
- ▶ Bounds on mixing time and rate of convergence to equilibrium
(among others)

Overview of the talk

Introduction

Convergence to equilibrium of the zero-range process

The zero-range process

Bound on mixing time and interpretation

Geometric structure

Setup

Distance \mathcal{W}

Ricci curvature for discrete processes

Modified log-Sobolev inequality

From mLSI to convergence to equilibrium

References

The zero-range process I

Consider K interacting particles on the complete graph with L sites.

The state space is $\mathcal{X}_{K,L} = \{\eta \in \mathbb{N}^L : \sum_i \eta_i = K\}$.

The zero-range process with **constant rates** can be described as:

1. Choose a site i uniformly at random
 - 1.1 If $\eta_i = 0$, do nothing
 - 1.2 Else, choose another site j uniformly at random and move 1 particle from i to j

$\eta^{i,j}$ denotes the new configuration after such a move.

$$Q_{K,L}(\eta, \theta) = \begin{cases} \frac{1}{L} & \theta = \eta^{i,j} \text{ for some } i, j \\ 0 & \text{else} \end{cases}$$

Invariant measure is the uniform measure $\pi_{K,L}$.

The zero-range process II

Good model for:

- ▶ Traffic-jam formation [Kaupužs et al., 2005]
- ▶ Population dynamics [Grange, 2020]
- ▶ Rewiring networks (e.g. Bianconi–Barabási model) [Grange, 2020], [Angel et al., 2005]
- ▶ ... any system in which deciding to move depends on the surroundings

Main result and interpretation

Convergence to equilibrium

The constant-rate zero range process with K particles and L sites has mixing time bounded by

$$\tau_{\text{mix}}(\varepsilon) \leq KL \log L \left(\frac{1}{8} - \frac{\log \varepsilon}{c} \right) \quad (1)$$

for some universal constant c .

* This is exponential convergence to equilibrium! *

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Setup

Finite space of states \mathcal{X} , irreducible, reversible Markov kernel Q and stationary measure π

$$Q(x, y)\pi(x) = Q(y, x)\pi(y)$$

Operator L acting on functions $\psi : \mathcal{X} \rightarrow \mathbb{R}$ is

$$L\psi(x) = \sum_{y \in \mathcal{X}} (\psi(y) - \psi(x))Q(x, y)$$

is the generator of a continuous time Markov chain.

Space of probability densities

$$\mathcal{P}(\mathcal{X}) := \left\{ \rho : \mathcal{X} \rightarrow \mathbb{R}_+ : \sum_{x \in \mathcal{X}} \rho(x) \pi(x) = 1 \right\}$$

Distance \mathcal{W}

We define a discrete transport distance, by analogy with the Wasserstein distance. For $\rho_0, \rho_1 \in \mathcal{P}(\mathcal{X})$,

$$\mathcal{W}(\rho_0, \rho_1)^2 := \inf_{\rho, \psi} \frac{1}{2} \int_0^1 \sum_{x, y \in \mathcal{X}} (\psi_t(x) - \psi_t(y))^2 \hat{\rho}_t(x, y) Q(x, y) \pi(x) dt$$

where the infimum runs over all sufficiently regular curves satisfying a continuity equation

$$\begin{cases} \frac{d}{dt} \rho_t(x) + \sum_{y \in \mathcal{X}} (\psi_t(y) - \psi_t(x)) \hat{\rho}_t(x, y) Q(x, y) = 0, & \forall x \in \mathcal{X}, \\ \rho|_{t=0} = \rho_0, \quad \rho|_{t=1} = \rho_1. \end{cases}$$

and $\hat{\rho}(x, y) := \theta(\rho(x), \rho(y))$ which is the logarithmic mean.

Markov semigroup as gradient flow

$$\mathcal{W}(\rho_0, \rho_1)^2 := \inf_{\rho, \psi} \frac{1}{2} \int_0^1 \sum_{x, y \in X} (\psi_t(x) - \psi_t(y))^2 \hat{\rho}_t(x, y) Q(x, y) \pi(x) dt$$

$$\text{s.t. } \frac{d}{dt} \rho_t(x) + \nabla \cdot (\hat{\rho}(x, y) \nabla \psi(x, y)) = 0$$

Endowing \mathcal{X} with this distance, we can interpret the Markov semigroup $P_t = e^{tL}$ as a gradient flow of Shannon's entropy

$$\mathcal{H}(\rho) := \sum_{x \in \mathcal{X}} \rho(x) \log \rho(x) \pi(x)$$

Ricci for discrete processes

Entropic Ricci curvature for discrete space

(\mathcal{X}, Q, π) has entropic Ricci curvature bounded from below by $\kappa \in \mathbb{R}$ if for any geodesic $\{\rho_t\}_{t \in [0,1]}$ on $(\mathcal{P}(\mathcal{X}), \mathcal{W})$ we have

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

In this case, we write $\text{Ric}(\mathcal{X}, Q, \pi) \geq \kappa$.

Ricci for the zero-range process (in brief)

In another contribution, M. Fathi and J. Maas provide explicit ways of computing bounds on Ricci for discrete processes

They show that for the ZRP with *increasing* rates, Ricci is positive

The ZRP with *constant* rates has $\text{Ric} \geq 0$

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The Modified log-Sobolev inequality I

Modified logarithmic Sobolev inequality

It is a **bound on the entropy** in terms of a norm of the gradient of our observable:

$$\mathcal{H}(\rho) \leq \frac{1}{2\lambda} \mathcal{I}(\rho) \quad (\text{mLSI}(\lambda))$$

where \mathcal{I} is the Fisher information

$$\mathcal{I}(\rho) := \int \rho |\nabla \log \rho|^2 d\pi = \|\nabla \log \rho\|_{\rho}^2$$

The Modified log-Sobolev inequality I

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mLSI for $\text{Ric} \geq 0$

If $\text{Ric}(\mathcal{X}, Q, \pi) \geq 0$ and the diameter of $(\mathcal{X}, d_{\mathcal{W}})$ is bounded by D , then the modified logarithmic Sobolev inequality ($\text{mLSI}(\lambda)$) holds with constant

$$\lambda = \frac{c}{D^2}$$

for some universal constant c .

The Modified log-Sobolev inequality II

The mLSI has many implications on convergence property, spectrum of the Laplacian and hypercontractivity

- * Our focus: mLSI implies entropy decay, which allows to bound the mixing time *

$$\mathcal{H}(P_t \rho) \leq e^{-2\lambda t} \mathcal{H}(\rho) \quad (\text{Entropy decay})$$

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From mLSI to entropy decay

$$\mathcal{H}(\rho) \leq \frac{1}{2\lambda} \mathcal{I}(\rho) \quad \rightarrow \quad \mathcal{H}(P_t \rho) \leq e^{-2\lambda t} \mathcal{H}(\rho)$$

When P_t is the heat semigroup,

$$\frac{d}{dt} \mathcal{H}(P_t \rho) = -\mathcal{I}(P_t \rho)$$

Hence

$$\mathcal{H}(P_t \rho) \leq -\frac{1}{2\lambda} \frac{d}{dt} \mathcal{H}(P_t \rho); \quad \frac{d}{dt} \mathcal{H}(P_t \rho) \leq -2\lambda \mathcal{H}(P_t \rho)$$

Using Gronwall's inequality, this yields an estimate on entropy decay

$$\mathcal{H}(P_t \rho) \leq e^{-2\lambda t} \mathcal{H}(\rho)$$

that quantifies convergence to equilibrium.

From entropy decay to bound on mixing time

Total variation mixing time of a Markov chain

Let P_t be the Markov semigroup on the space of densities $\mathcal{P}(\mathcal{X})$ and P_t^* be its dual acting on probability measures.

For $\varepsilon > 0$,

$$\tau_{\text{mix}}(\varepsilon) := \inf \left\{ t > 0 : \|P_t^* \delta_x - \pi\|_{TV} < \varepsilon \quad \forall x \in \mathcal{X} \right\}$$

From entropy decay to bound on mixing time

Total variation mixing time of a Markov chain

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→ Relation to entropy:

Pinsker's inequality

Let μ be a probability distribution and π be the uniform distribution over \mathcal{X} . Then

$$\|\rho - \pi\|_{TV}^2 \leq \frac{1}{2}\mathcal{H}(\rho) \quad (\text{Pinsker})$$

From entropy decay to bound on mixing time I

Ingredients:

1. Bound on \mathcal{H} in terms of the diameter: $\mathcal{H}(P_t \rho) \leq \frac{\mathcal{W}^2(\rho, 1)}{4t}$
2. Pinsker's: $\|P_t \rho - 1\|_{TV}^2 \leq \frac{1}{2} \mathcal{H}(P_t \rho)$
3. Entropy decay: $\mathcal{H}(P_t \rho) \leq e^{-2\lambda t} \mathcal{H}(\rho)$

From (1) we obtain $\mathcal{H}(P_t \rho) \leq 2$ for

$$t \geq \frac{D^2}{8} := t_0 \quad (\text{bound } \#1)$$

Plug this into (2) and combine with (3) to obtain

$$\|P_t \rho - 1\|_{TV} \leq \sqrt{\frac{1}{2} \mathcal{H}(P_t \rho)} \leq \sqrt{\frac{1}{2} e^{-2\lambda t} \mathcal{H}(P_{t_0} \rho)} \leq e^{-\lambda t}$$

We get ε -closeness for

$$t \geq -\frac{\log \varepsilon}{\lambda} \quad (\text{bound } \#2)$$

From entropy decay to bound on mixing time II

Ingredients:

1. Bound on \mathcal{H} in terms of the diameter: $\mathcal{H}(P_t \rho) \leq \frac{\mathcal{W}^2(\rho, 1)}{4t}$
2. Pinsker's: $\|P_t \rho - 1\|_{TV}^2 \leq \frac{1}{2} \mathcal{H}(P_t \rho)$
3. Entropy decay: $\mathcal{H}(P_t \rho) \leq e^{-2\lambda t} \mathcal{H}(\rho)$

Sum the two bounds $t \geq D^2/8$ and $t \geq \log \varepsilon / \lambda$ to obtain an upper bound on the mixing time

$$\tau_{\text{mix}} \leq \frac{1}{8} D^2 - \frac{\log \varepsilon}{\lambda}$$

Bound on the mixing time of the zero-range process

$$\tau_{\text{mix}} \leq \frac{1}{8} D^2 - \frac{\log \varepsilon}{\lambda}$$

Recall: The ZRP has $\text{Ric}(\mathcal{X}_{KL}, Q_{KL}, \pi_{KL}) \geq 0$, hence a mLSI with constant $\lambda = \frac{c}{D^2}$ holds

Moreover: There exists a constant $c > 0$ such that for any L, K

$$D_{KL} \leq cK\sqrt{L \log L}$$

Convergence of the ZRP

The total variation mixing time of the zero range process on $\mathcal{X}_{K,L}$ with constant uniform rates is

$$\tau_{\text{mix}}(\varepsilon) \leq KL \log L \left(\frac{1}{8} - \frac{\log \varepsilon}{c} \right)$$

for some universal constant c .

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Discussion

- ▶ The main contribution of this paper for the ZRP is a *quantification* of its convergence ([Andjel et al., 2000])
- ▶ The dependence on the diameter is optimal, since it is sharp (up to the values of the constant) for the random walk on the one-dimensional discrete torus
- ▶ However, the mLSI constant for ZRP is not believed to be optimal: dependence of curvature on D in high dimensions is not optimal (Gaussian concentration instead)
- ▶ Developments in this sense: [Münch, 2023], [Brannan et al., 2020]

Some examples of other applications I

mLSI constant (and Poincaré) and implied convergence rate for:

- ▶ Bernoulli-Laplace model (diffusion of two incompressible gases)
- ▶ Random transposition model (random permutations) [Caputo et al., 2007]
- ▶ Hard-core models (nearest-neighbour exclusion)
- ▶ Glauber dynamics (Ising model) [Erbar et al., 2017]

Additional formulas I

Distance $d_{\mathcal{W}}$ on \mathcal{X}

The distance \mathcal{W} on $\mathcal{P}(\mathcal{X})$ induces a distance on \mathcal{X} by restricting to Dirac masses, i.e. for $x, y \in \mathcal{X}$

$$d_{\mathcal{W}}(x, y) := \mathcal{W}(\delta_x, \delta_y)$$

Induced Riemannian structure on \mathcal{X}

$$(\Psi, \Phi)_\rho := \frac{1}{2} \sum_{x,y} \Psi(x, y) \Phi(x, y) \hat{\rho}(x, y) Q(x, y) \pi(x)$$

Additional formulas II

Discrete gradient and divergence

$$\nabla\psi(x, y) = \psi(y) - \psi(x)$$

$$\begin{aligned}\nabla \cdot (\nabla\psi)(x) &= \frac{1}{2} \sum_y (\nabla\psi(x, y) - \nabla\psi(y, x)) Q(x, y) \\ &= \frac{1}{2} \sum_y (\psi(y) - \psi(x) - \psi(x) + \psi(y)) Q(x, y) \\ &= \sum_y (\psi(y) - \psi(x)) Q(x, y)\end{aligned}$$

Additional formulas III

Heat flow as gradient flow of entropy

Heat equation $\rho'_t = \Delta \rho_t = \nabla \cdot \nabla \rho_t$

Continuity equation $\rho'_t + \nabla \cdot (\hat{\rho} \nabla \psi) = 0$

The heat equation can be re-written as a continuity equation if

$$\nabla \psi_t = -\frac{\nabla \rho_t}{\hat{\rho}_t}$$

The gradient of the entropy is $\text{grad}_{\mathcal{W}} \mathcal{H}(\rho_t) = \nabla \log \rho_t$

Hence, we get that the heat flow is the gradient flow of the entropy if

$$\nabla \psi_t = -\frac{\nabla \rho_t}{\hat{\rho}_t} = -\nabla \log \rho_t;$$

which gives

$$\frac{\nabla \rho_t}{\hat{\rho}_t} = \nabla \log \rho_t \tag{2}$$

i.e. precisely that $\hat{\rho}_t$ is the logarithmic mean.