MLSI: Theory, Examples and Consequences Lecture 3

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DISCRETE CURVATURE AND CONJECTURES

2 SLC and Matroid Bases Exchange

BOCHNER-BAKRY-ÉMERY CRITERION

The following 2nd derivative criterion is also useful, and inspires a notion of *discrete curvature*, mimicking the Ricci curvature.

Proposition (Bochner'46, Lichnérowicz'58)

$$\inf_{f} \frac{\mathcal{E}(f,f)}{\operatorname{Var}_{\pi} f} =: \lambda = \inf_{f} \frac{\mathcal{E}(-Lf,f)}{\mathcal{E}(f,f)} =: \mu_{P} =: \mu.$$

Proof. $\lambda \leq \mu$: Use Cauchy-Schwartz. Indeed, w/ $\mathbb{E}_{\pi}f = 0$,

$$\begin{split} \mathcal{E}(f,f) &= \mathbb{E}(f(-Lf)) &\leq \left(\operatorname{Var}_{\pi} f \right)^{1/2} \left(\mathbb{E}(-Lf)^{2} \right)^{1/2} \\ &\leq \frac{1}{\sqrt{\lambda}} (\mathcal{E}(f,f))^{1/2} \left(\mathbb{E}(-Lf)^{2} \right)^{1/2} \\ &= \frac{1}{\sqrt{\lambda}} (\mathcal{E}(f,f))^{1/2} \left(\mathcal{E}(-Lf,f) \right)^{1/2}. \end{split}$$

BOCHNER-BAKRY-ÉMERY CRITERION (CONTD.)

Other direction, $\lambda \geq \mu$: 2nd derivative and integration. Starting with

$$\frac{d}{dt}\mathrm{Var}(H_tf) = -2\mathcal{E}(H_tf,H_tf) \text{ and } \frac{d}{dt}\mathcal{E}(H_tf,H_tf) = -2\mathcal{E}(H_tf,-LH_tf)\,.$$

Observe that as $t \to \infty$, $H_t f \to \mathbb{E}_\pi f$, and so $\mathcal{E}(H_t f, H_t f) \to 0$. Hence,

$$\mathcal{E}(f,f) = -\int_0^\infty \frac{d}{dt} \mathcal{E}(H_t f, H_t f) dt = 2 \int_0^\infty \mathcal{E}(H_t f, -L(H_t f)) dt$$

$$= 2 \int_0^\infty \mathcal{E}(-L^*(H_t f), H_t f) dt \ge 2\mu_{P^*} \int_0^\infty \mathcal{E}(H_t f, H_t f) dt$$

$$= -\mu_{P^*} \int_0^\infty \frac{d}{dt} \operatorname{Var}(H_t f) dt = \mu_{P^*} \operatorname{Var} f,$$

implying that $\lambda_P = \lambda_{P^*} \geq \mu_P$.



MLSI AND BAKRY-ÉMERY CRITERION

What about repeating the above for the entropy constant?

Proposition (Bakry-Émery'85)

$$\inf_{f>0} \frac{\mathcal{E}(f,\log f)}{\operatorname{Ent}_{\pi} f} =: \alpha \ge \inf_{f>0} \frac{u(f)}{\mathcal{E}(f,\log f)},$$

where
$$u(f) = \mathcal{E}(-Lf, \log f) + \mathcal{E}(f, (-Lf)/f)$$
.

Some relevant references include:

[Boudou, Caputo, Dai Pra, Posta, 2005]. "Spectral gap estimates for interacting particle systems via a Bochner type identity," J. Funct. Analysis.

[M. Erbar, J. Maas, P.T. 2015]. "Discrete Curvature Bounds for Bernoulli-Laplace and Random Transposition Models," Annales Fac. Sci. Toulouse.

Bochner formula (iterated gradient Γ_2 criterion) : application: discrete Buser ...

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DEFINITION [BOCHNER W/ PARAMETER K]

Curvature of G is at least K, if $\forall f: V \to \mathbb{R}$, and $\forall x \in V$,

$$\Delta\Gamma(f,f)(x) - 2\Gamma(f,\Delta f)(x) \geq K \Gamma(f,f)(x),$$

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where

$$\Delta f(x) = \sum_{y:(x,y)\in E} (f(y) - f(x)).$$

And given $f, g: V \to \mathbb{R}$, also define:

$$\Gamma(f,g)(x) = \frac{1}{2} \sum_{y:(x,y) \in E} (f(x) - f(y))(g(x) - g(y)).$$

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Note:
$$\Gamma(f)(x) := \Gamma(f, f)(x) = \frac{1}{2} \sum_{y:(x,y) \in E} (f(x) - f(y))^2 =: |\nabla f(x)|^2$$
.

Γ₂ CALCULUS

Basically, using the iterated gradient:

$$2\Gamma_2(f,g) = \Delta\Gamma(f,g) - \Gamma(f,\Delta g) - \Gamma(\Delta f,g)$$
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Γ_2 Calculus

EQUIVALENTLY ...

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Γ_2 CALCULUS (CONTD.)

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$$2\Gamma_{2}(f)(x) = \Delta\Gamma(f)(x) - 2\Gamma(f, \Delta f)(x)$$

$$= \sum_{v \sim x} \Gamma(f)(v) - d(x)\Gamma(f)(x) - \sum_{v \sim x} f(v)(\Delta f(v) - \Delta f(x))$$

$$= \left(\sum_{v \sim x} f(v)\right)^{2} - \frac{d(x)}{2} \sum_{v \sim x} f^{2}(v) + \sum_{u \sim v \sim x} \frac{f^{2}(u) - 4f(u)f(v) + 3f^{2}(v)}{2}$$

$$= \left(\sum_{v \sim x} f(v)\right)^{2} - \sum_{v \sim x} \frac{d(x) + d(v)}{2} f^{2}(v) + \frac{1}{2} \sum_{u \sim v \sim x} \left((f(u) - 2f(v))^{2}\right).$$
(2.1)

Γ_2 Calculus (contd.)

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(2.1)

For *d*-regular, further simplifies to:

$$2\Gamma_2(f)(x) = d\sum_{v \sim x} f^2(v) + \left(\sum_{v \sim x} f(v)\right)^2 + \sum_{v \sim x} \sum_{u \sim v} \left(\frac{f^2(u)}{2} - 2f(u)f(v)\right).$$

(2.2)

Cheeger is tight if curvature > 0

 $h := h(G) := \min_{A \subset V} |\partial A|/|A|$, the Cheeger const, of G; $\lambda > 0$: gap(G).

THEOREM (A-M, L-S, J-S 80's)

$$\frac{h^2}{c_1 \operatorname{maxdeg}(G)} \le \lambda \le c_2 h.$$

THEOREM (KLARTAG-KOZMA-RALLI-T. '14)

1. Bochner w/ parameter K implies: for any subset $A \subset V$,

$$|\partial A| \geq \frac{1}{2} \min \Bigl\{ \sqrt{\lambda}, \frac{\lambda}{\sqrt{2|K|}} \Bigr\} \; |A| \Bigl(1 - \frac{|A|}{|V|} \Bigr) \,.$$

2. Bochner w/ parameter $K \ge 0$ implies $\lambda \ge K$, and hence:

$$\lambda \leq 16h^2$$
.

3. Abelian Cayley graphs satisfy Bochner w/ parameter $K \ge 0$.

$CD(K, \infty)$ WITH $K \ge 0$: Examples

- 1. Complete graph K_n : Curvature = 1 + n/2.
- 2. Discrete *n*-cube Q_n : Curvature = 2.
- 3. Symmetric group S(n) with the transposition metric: Curvature = 2
- 4. **General Proposition**. If T is the maximum number of triangles containing any edge, then $K \le 2 + T/2$.
- 5. **Abelian necessary!** On S_n , the (left) Cayley graph generated by $(12), (12...n) \pm 1$, the Cheeger constant is $c_1 n^{-2}$, while the spectral gap is $c_2 n^{-3}$, with $c_1, c_2 > 0$, independent of n.

Cheeger, $CD(K, \infty)$ with $K \ge 0$

- Qn. 1 Can we characterize the graphs or Markov kernels which satisfy non-negative curvature?
- Qn. 2 Can we characterize the graphs for which the Cheeger inequality is tight?
- Qn. 3 More examples? Non-crossing partition lattice NC(n)?

OLLIVIER-VILLANI

"In positive curvature, balls are closer than their centers."

Coarse Ricci: Take two small balls and compute the transportation distance between them. If it is smaller than the distance between the centers of the balls, then coarse Ricci is *positive*.

$$W_1(\mu_x,\mu_y)=:(1-\kappa(x,y))d(x,y),$$

Examples.

- **1**. *n*-cube: μ_x uniform on the n+1 neighbors of x (including itself). For x, y, neighbors, $\kappa(x, y) = 2/(n+1)$.
- **2**. S_n with transpositions: For σ, τ differing in a transposition, $\kappa(x,y) = 1/\binom{n}{2}$.



(Coarse) Ricci of Hypercube

Proposition (folklore)

The n-cube has coarse Ricci = 2/(n+1).

Proof sketch.

- (i) Consider the *lazy* random walk on the *n*-cube.
- (ii) Use a simple (path) coupling argument to show that two copies of the chain started at *neighboring vertices* $x, y \in \{0,1\}^n$ can be "coupled" with probability at least 2/(n+1) in one step.

(Coarse) Ricci of Transposition Graph

Proposition

 S_n with transpositions has coarse Ricci = $1/\binom{n}{2}$.

Proof sketch.

Lower bound:

- (i) Consider the *lazy* random transposition chain on S_n .
- (ii) Use a simple (path) coupling argument to show that two copies of the chain started at $\sigma, \tau \in S_n$ with $d(\sigma, \tau) = 1$, can be coupled with probability at least $1/\binom{n}{2}$ in one step.

Upper bound: Follows by showing that there is no better coupling – use (Kantorovich's) dual formulation of W_1 :

$$W_1(\nu,\mu) = \sup_{f: 1-\text{Lip}} \left(\mathcal{E}_{\nu} f - \mathcal{E}_{\mu} f \right).$$



Peres-Tetali "Conjecture"!

Does coarse Ricci at least $\kappa > 0$ imply the MLSI constant $\alpha \geq \kappa$?

Something weaker is known: namely that a W_1 transport-Entropy inequality follows, thanks to (Marton??, Eldan, Lehec, Lee'16)

MLSI FOR BASES EXCHANGE WALK

I am thankful to Heng Guo for letting me borrow some of his slides in this section.

MATROID

A matroid $\mathcal{M} = (E, \mathcal{I})$ consists of a finite ground set E and a collection \mathcal{I} of subsets of E (independent sets) such that:

- $\emptyset \in \mathcal{I}$:
- if $S \in \mathcal{I}$, $T \subseteq S$, then $T \in \mathcal{I}$ (downward closed);
- if $S, T \in \mathcal{I}$ and |S| > |T|, then there exists an element $i \in S \setminus T$ such that $T \cup \{i\} \in \mathcal{I}$ (augment axiom).

Maximum independent sets are the bases.

For any two bases, there is a sequence of exchanges of ground set elements that take one basis to the other.

Let n = |E| and r be the rank, namely the size of any basis.

Bases-exchange walk

The following Markov chain $P_{\text{BX},\pi}$ converges to a "homogeneous SLC" π :

- remove an element uniformly at random from the current basis (call the resulting set *S*);
- **2** add $i \notin S$ with probability proportional to $\pi(S \cup \{i\})$.

The implementation of the second step may be non-trivial.

MLSI FOR MATROID BASIS EXCHANGE

THEOREM (MARY CRYAN-HENG GUO-GIORGOS MOUSA)

For any $f:\Omega\to\mathbb{R}_{\geq 0}$,

$$\mathcal{E}_{P_{\mathsf{BX},\pi}}(f,\log f) \geq rac{1}{r} \cdot \mathsf{Ent}_{\pi}(f),$$

where r is the rank of the matroid.

Many open problems remain!

- Sampling spanning trees of G with no broken circuit the same as evaluation $T_G(1,0)$ of the Tutte polynomial, leading coefficient $|a_1[\chi_G(\lambda)]|$ of the chromatic polynomial (up to sign), number of maximum G-parking functions, sampling acyclic orientations with a unique sink ...
- Sampling all acyclic orientations of G
- Negative correlation for random forests of G
- (More generally) characterization of matroids with negative correlation for random bases.

STRONGLY LOG-CONCAVE POLYNOMIALS

Log-concave Polynomial

A polynomial $p \in \mathbb{R}_{\geq 0}[x_1, \dots, x_n]$ is log-concave (at **x**) if the Hessian $\nabla^2 \log p(\mathbf{x})$ is negative semi-definite.

 \Rightarrow $\nabla^2 p(\mathbf{x})$ has at most one positive eigenvalue.

STRONGLY LOG-CONCAVE POLYNOMIAL

A polynomial $p \in \mathbb{R}_{\geq 0}[x_1, \dots, x_n]$ is strongly log-concave if for any index set $I \subseteq [n]$, $\partial_I p$ is log-concave at $\mathbf{1}$.

Originally introduced by Gurvits (2009), equivalent to:

- Completely log-concave (Anari, Oveis Gharan, and Vinzant, 2018);
- Lorentzian polynomials (Brändén and Huh, 2019+).



STRONGLY LOG-CONCAVE DISTRIBUTIONS

A distribution $\pi:2^{[n]}\to\mathbb{R}_{\geq 0}$ is strongly log-concave if so is its generating polynomial

$$g_{\pi}(\mathbf{x}) = \sum_{S \subseteq [n]} \pi(S) \prod_{i \in S} x_i.$$

An important example of homogeneous strongly log-concave distributions is the uniform distribution over bases of a matroid (Anari, Oveis Gharan, and Vinzant 2018; Brändén and Huh 2019+).

ALTERNATIVE CHARACTERIZATION FOR SLC

Brändén and Huh (2019+): An r-homogeneous multiaffine polynomial p with non-negative coefficients is strongly log-concave if and only if:

- the support of *p* is the bases of some matroid;
- after taking r-2 partial derivatives, the quadratic is real stable or $\mathbf{0}$.

Real stable: $p(\mathbf{x}) \neq 0$ if $\Im(x_i) > 0$ for all i.

Real stable polynomials (and strongly Rayleigh distributions) capture only "balanced" matroids, whereas SLC polynomials capture all matroids.



Bases-exchange walk

The following Markov chain $P_{\mathrm{BX},\pi}$ converges to a homogeneous SLC π :

- remove an element uniformly at random from the current basis (call the resulting set *S*);
- **2** add $i \notin S$ with probability proportional to $\pi(S \cup \{i\})$.

The implementation of the second step may be non-trivial.

Recall the mixing time defn.

$$t_{\mathsf{mix}}(P,\varepsilon) := \min_{t} \left\{ t \mid \|P^{t}(x_{0},\cdot) - \pi\|_{\mathsf{TV}} \le \varepsilon \right\}.$$

THEOREM (CRYAN-GUO-MOUSA 2019)

For any r-homogeneous strongly log-concave distribution π ,

$$t_{\mathsf{mix}}(P_{\mathsf{BX},\pi},\varepsilon) \le r\left(\log\log\frac{1}{\pi_{\mathsf{min}}} + \log\frac{1}{2\varepsilon^2}\right),$$

where $\pi_{\min} = \min_{x \in \Omega} \pi(x)$.

Previously, Anari, Liu, Oveis Gharan, and Vinzant (2019):

$$t_{\mathsf{mix}}(P_{\mathsf{BX},\pi},\varepsilon) \le r\left(\log\frac{1}{\pi_{\mathsf{min}}} + \log\frac{1}{\varepsilon}\right)$$

E.g. for the uniform distribution over bases of matroids (with n elements and rank r), the new bound is $O(r(\log r + \log \log n))$, whereas the previous bound is $O(r^2 \log n)$.

LEVELS OF INDEPENDENT SETS

The set of all independent sets of a matroid \mathcal{M} is downward closed.

Let $\mathcal{M}(k)$ be the set of independent sets of size k. Thus, $\mathcal{M}(r)$ is the set of all bases.

Let \mathcal{M}_i denote the matroid \mathcal{M} after contracting i, which is another matroid itself.

WEIGHTS FOR INDEPENDENT SETS

Equip ${\mathcal M}$ with the following inductively defined weight function:

$$w(I) := \begin{cases} \pi(I)Z_r & \text{if } |I| = r, \\ \sum_{I' \supset I, \ |I'| = |I| + 1} w(I') & \text{if } |I| < r, \end{cases}$$

for some normalization constant $Z_r > 0$.

For example, we may choose w(B) = 1 for all $B \in \mathcal{B}$ and $Z_r = |\mathcal{B}|$, which corresponds to the uniform distribution over \mathcal{B} .

Let π_k be the distribution such that $\pi_k(I) \propto w(I)$, and Z_k be the corresponding normalizing constant.

DIFFERENT VIEWS

- Polynomial: $\frac{\partial \mathbf{p}}{\partial x_i}$; setting $x_i = 0$; $(r k)! \frac{\partial}{\partial x_i} \mathbf{p}(\mathbf{1})$
- Matroid: contraction over i; deletion of i; w(I)
- Distribution: conditioning on having i; conditioning on not having i; proportional to $\pi_k(I)$

RANDOM WALK BETWEEN LEVELS

There are two natural random walks converging to π_k .

The "down-up" random walk P_k^{\vee} :

- \rightarrow 1. remove an element of $I \in \mathcal{M}(k)$ uniformly at random to get $I' \in \mathcal{M}(k-1)$;
 - 2. move to J such that $J \in \mathcal{M}(k), J \supset I'$ with probability $\frac{w(J)}{w(I')}$.

The bases-exchange walk $P_{\text{BX},\pi} = P_r^{\vee}$.

The "up-down" walk P_k^{\wedge} is defined similarly.

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The "up-down" walk P_k^{\wedge} is defined similarly.

Let A_k be the matrix whose rows are indexed by $\mathcal{M}(k)$ and columns by $\mathcal{M}(k+1)$ such that $A_k(I,J)=1$ if and only if $I\subset J$.

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$$\mathbf{w}_k = \{w(I)\}_{I \in \mathcal{M}(k)}$$
, and

$$P_{k+1}^{\downarrow} := rac{1}{k+1} \cdot A_k^{\mathrm{T}};$$
 $P_k^{\uparrow} := \operatorname{diag}(\mathbf{w}_k)^{-1} A_k \operatorname{diag}(\mathbf{w}_{k+1}).$

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We have

$$\begin{split} P_{k+1}^{\vee} &= P_{k+1}^{\downarrow} P_{k}^{\uparrow}; \\ P_{k}^{\wedge} &= P_{k}^{\uparrow} P_{k+1}^{\downarrow}. \end{split}$$

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KEY LEMMA

LEMMA

For any
$$k \geq 2$$
 and $f: \mathcal{M}(k) \to \mathbb{R}_{\geq 0}$,

$$\frac{\mathsf{Ent}_{\pi_k}(f)}{k} \geq \frac{\mathsf{Ent}_{\pi_{k-1}}(P_{k-1}^\uparrow f)}{k-1}.$$

KEY LEMMA

LEMMA

For any $k \geq 2$ and $f : \mathcal{M}(k) \to \mathbb{R}_{>0}$,

$$\frac{\mathsf{Ent}_{\pi_k}(f)}{k} \geq \frac{\mathsf{Ent}_{\pi_{k-1}}(P_{k-1}^{\uparrow}f)}{k-1}.$$

- ullet Applying P_{k-1}^{\uparrow} to the left corresponds to the random walk P_k^{\downarrow} .
- The lemma asserts that P_k^{\downarrow} contracts the relative entropy by at least (1-1/k):

$$\operatorname{Ent}_{\pi_{k-1}}(P_{k-1}^{\uparrow}f) \leq (1-1/k)\operatorname{Ent}_{\pi_k}(f)$$
.



BASE CASE

For the base case, we want to show that

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Using $a \log \frac{a}{b} \ge a - b$ for a, b > 0, we can get

$$\mathsf{Ent}_{\pi_2}(f) - 2\mathsf{Ent}_{\pi_1}(P_1^{\uparrow}f) \geq 1 - \frac{1}{2Z_2} \cdot h^{\mathsf{T}}Wh,$$

where $W_{ij} = w(\{i,j\})$ and $h = P_1^{\uparrow} f$.

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$$\operatorname{\mathsf{Ent}}_{\pi_2}(f) - 2\operatorname{\mathsf{Ent}}_{\pi_1}(P_1^\uparrow f) \geq 1 - \frac{1}{2Z_2} \cdot h^{\operatorname{\mathtt{T}}} W h,$$

where $W_{ij} = w(\{i,j\})$ and $h = P_1^{\uparrow} f$.

Since $W = (r-2)!Z_r\nabla^2 g_{\pi}(\mathbf{1})$, it has at most one positive eigenvalue. The quadratic form is maximized at $h = P_1^{\uparrow} f = \mathbf{1}$, which helps prove the base case...



Bound the mixing time directly

For a distribution τ on $\mathcal{M}(k)$, the relative entropy $D(\tau \parallel \pi_k) = \operatorname{Ent}_{\pi_k}(D_k^{-1}\tau)$ where $D_k = \operatorname{diag}(\pi_k)$. Moreover, after one step of P_k^\vee , the distribution is $(\tau^{\mathrm{T}}P_k^\vee)^{\mathrm{T}} = (P_k^\vee)^{\mathrm{T}}\tau$. Since P_k^\vee is reversible, $D_k^{-1}(P_k^\vee)^{\mathrm{T}} = P_k^\vee D_k^{-1}$.

$$\begin{split} D\left((P_k^\vee)^\mathrm{T}\tau \parallel \pi_k\right) &= \mathrm{Ent}_{\pi_k}(D_k^{-1}(P_k^\vee)^\mathrm{T}\tau) \\ &= \mathrm{Ent}_{\pi_k}(P_k^\vee D_k^{-1}\tau) \\ &= \mathrm{Ent}_{\pi_k}(P_k^\vee P_{k-1}^\uparrow D_k^{-1}\tau) \\ &\leq \mathrm{Ent}_{\pi_{k-1}}(P_{k-1}^\uparrow D_k^{-1}\tau) \\ &\leq \left(1 - \frac{1}{k}\right) \mathrm{Ent}_{\pi_k}(D_k^{-1}\tau) \\ &= \left(1 - \frac{1}{k}\right) D\left(\tau \parallel \pi_k\right). \end{split} \tag{Jensen's inequality}$$

The mixing time bound follows from Pinsker's inequality

$$2\|\tau - \sigma\|_{\mathsf{TV}}^2 \le D(\tau \parallel \sigma).$$



Many open problems remain!

- Sampling spanning trees of G with no broken circuit the same as evaluation $T_G(1,0)$ of the Tutte polynomial, leading coefficient $|a_1[\chi_G(\lambda)]|$ of the chromatic polynomial (up to sign), number of maximum G-parking functions, sampling acyclic orientations with a unique sink ...
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- (More generally) characterization of matroids with negative correlation for random bases.

FIN

Thank you!