The Li-Yau Inequality and the Geometry of Graphs

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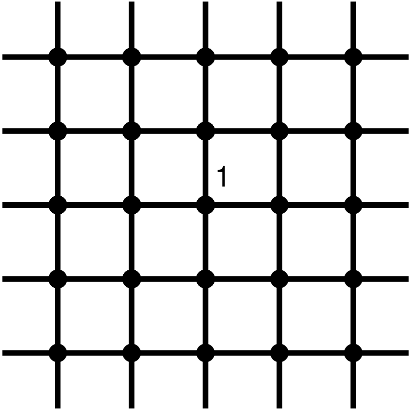
Understanding random walks:



Lazy random walk - stay in place with prob. $\frac{1}{2}$

What to study: distribution of random walk over time.

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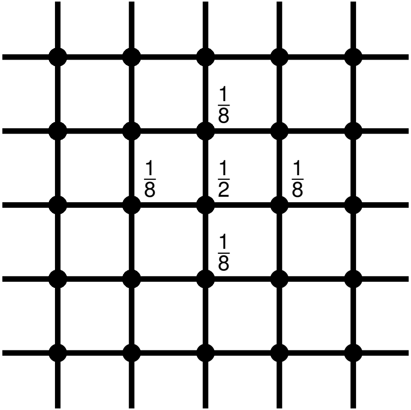

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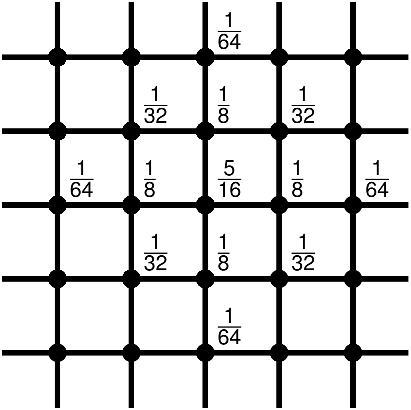

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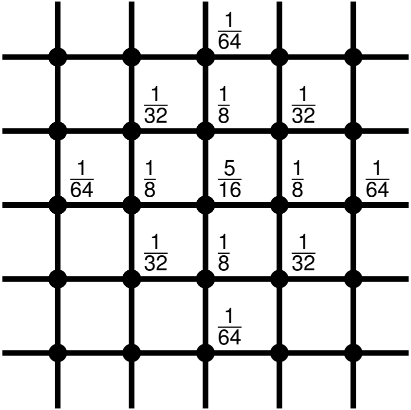

Behavior of random walk: Governed by shape of graph.

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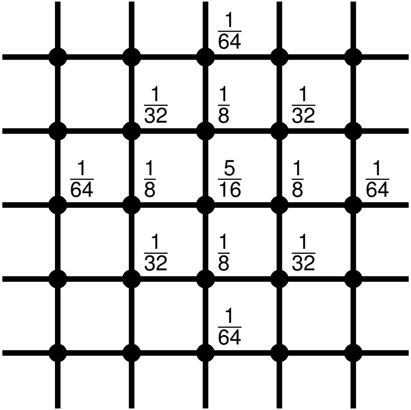

Basic Question: How to understand diffusion of random walks by geometric means and vice versa

Lazy random walk:

- Stay in place each step with probability $\frac{1}{2}$.
- $\Rightarrow$ time in place geometrically distributed
- Staying in place makes distribution better behaved

Continuous time random walk:

- Stay in place for *exponential time*
- Distribution is similarly well behaved
- Distribution $u(x,t)$ over time:

$$u(x,t) = \left(\left(D e^{t\Delta} D^{-1} \right) u(\cdot, 0) \right)(x)$$

- *Very* closely related to heat equation $\frac{\partial}{\partial t} u = \Delta u$.

Focus for talk: Understanding positive solutions to heat equation

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Focus for talk: Understanding positive solutions to heat equation

Harnack Inequalities

Goal: Given u positive solution to heat equation on G, understand evolution of u.

- Harnack inequality: Given (x, t_1), (y, t_2) with $t_2 \geq t_1$ and positive solution to the heat equation u bound

$$\frac{u(x, t_1)}{u(y, t_2)} < C$$

  where C depends on $|t_2 - t_1|$, $d(x, y)$.
- Gold Standard: If $|d(x, y)| < R$, and $|t_2 - t_1| < R^2$, then C can be taken to be an absolute constant.

Harnack inequalities

Harnack inequalities: Powerful tools, but...

- How do verify that they hold?
- Delmotte: Showed the following are equivalent (on graphs):
  - Poincaré inequality + volume doubling (eigenvalue inequality + volume growth estimate)
  - Gaussian bounds on heat kernel.
  - (Parabolic) Harnack inequality
- Grigor'yan and Saloff-Coste: same in Riemannian manifold case (earlier)

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Remark: Result shows symbiotic nature of results connecting distribution of RW and geometry.

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Hard to check! Simple condition to guarantee?
In manifold case: curvature.

Gradient estimates

Local condition implying Harnack?

Li-Yau Inequality (simple form)

Suppose M is a compact n dimensional manifold with non-negative curvature. If u is a positive solution to the heat equation on M for $t \leq T$, then for every $x \in M$

$$\frac{|\nabla u|^2}{u^2}(x,t) - \frac{u_t}{u}(x,t) \leq \frac{n}{2t}.$$

at all points (x, t)

Integrating gradient estimates: Proves Harnack inequality.

Note: More general form for more general operators/non-compact case/negative curvature bound/etc...

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Goal

- Goal: Understand evolution of positive solutions from *local* information – can yield global information on graph geometry.
- Want: Analogue of Li-Yau inequality for positive solutions to heat equation on graphs.
- Need: Understand discrete analogues of many important ideas on graphs:
  - Gradient of functions?
  - Curvature/Dimension?
  - ...

Gradients on Graphs

Bakry-Emery gradient operators:

For functions $f, g : V(G) \to \mathbb{R}$

$$(\Delta f)(x) = \frac{1}{d_x} \sum_{y \sim x} (f(y) - f(x))$$

Key property: In continuous case

$$\Delta(fg) = f\Delta g + g\Delta f + 2\langle \nabla f, \nabla g \rangle$$

Gradients on Graphs

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$$(\Delta f)(x) = \frac{1}{d_x} \sum_{y \sim x} (f(y) - f(x))$$

$$\begin{aligned}\Gamma(f,g)(x) &= \frac{1}{2}\left(\Delta(fg) - f\Delta g - g\Delta f\right) \\ &= \frac{1}{2d_x} \sum_{y \sim x} (f(y) - f(x))(g(y) - g(x)) = \langle \nabla f, \nabla g \rangle \\ \Gamma(f) &= \Gamma(f,f) = |\nabla f|^2\end{aligned}$$

Gradients on Graphs

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$$= \frac{1}{2d_x} \sum_{y \sim x} (f(y) - f(x))(g(y) - g(x)) = \langle \nabla f, \nabla g \rangle$$

$$\Gamma(f) = \Gamma(f,f) = |\nabla f|^2$$

$$\Gamma_2(f) = \frac{1}{2}(\Delta\Gamma(f) - 2\Gamma(f, \Delta f))$$

Graph curvature

An n-dimensional manifold M with curvature $\geq -K$ satisfies the

Bochner Formula

For every smooth function $f : M \to \mathbb{R}$

$$\frac{1}{2}(\Delta|\nabla f|^2 - 2\langle \nabla f, \nabla \Delta f \rangle) \geq \frac{1}{n}(\Delta f)^2 - K|\nabla f|^2$$

at every point x.

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Observation: Bochner formula real application of curvature in Li-Yau proof

From work of Bakry, Emery: Satisfying Bochner formula can be used as it definition of curvature in many settings.

Graph curvature

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at every point x.

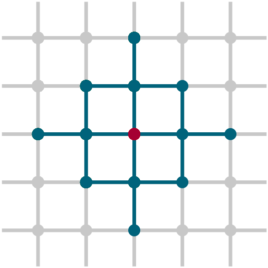
A graph G satisfies the curvature-dimension inequality $CD(n, -K)$ if

$$\Gamma_2(f) = \frac{1}{2}(\Delta\Gamma(f) - 2\Gamma(f, \Delta f)) \geq \frac{1}{n}(\Delta f)^2 - K|\Gamma(f)|^2$$

for every function f.

Curve ball

- Every graph satisfies $CD(2, -1 + \frac{1}{\max \deg(v)})$.
- Graphs satisfying $CD(n, 0)$ for some n: certain Cayley graphs of polynomial growth.
- Local property: Need to check distance two neighborhoods of vertices.



Challenges:

Continuous mathematics? Too easy!

Li-Yau proof:

- Uses maximum principle: Pick some function H to maximize and at maximum:

$$\Delta H \leq 0 \qquad \frac{\partial}{\partial t} H \geq 0 \qquad \nabla H = 0$$

- Discrete: No reasonable definition of ∇ so that $\nabla H = 0$
- Continuous case: Look at $\log u$ instead of u.

$$\Delta(\log u) = \frac{|\nabla u|^2}{u^2} - \frac{\Delta u}{u} = |\nabla \log u|^2 - (\log u)_t.$$

- Discrete: Royal mess!

$$\Delta(\log u)(x) = \frac{1}{d_x} \sum_{y \sim x} \log\left(\frac{y}{x}\right) = ???$$

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Deforestation:

How to get rid of log?

- Key to Li-Yau proof: If $f = \log u$

$$\Delta f = |\nabla f|^2 - f_t$$

  Not true at all in discrete case! (No reasonable inequalities, even!)

- Why important? Bochner formula:

$$\frac{1}{2}(\Delta|\nabla f|^2 - 2\langle \nabla f, \nabla \Delta f\rangle) \geq \frac{1}{n}(\Delta f)^2$$

  Relates $\Delta|\nabla f|^2$ and $(\Delta f)^2 = (|\nabla f|^2 - f_t)^2$.

- Discrete case: Need new identity.

Searching for an identity

What can replace $\Delta(\log u) = -|\nabla \log u| + \frac{\Delta u}{u}$?

Infinite family of identities: On manifolds

$$\Delta u^p = pu^{p-1}\Delta u + \frac{p-1}{p} u^{-p}|\nabla u^p|^2$$

Key fact: Identity holds for graphs for $p = \frac{1}{2}$:

$$-2\sqrt{u}\Delta\sqrt{u} = 2\Gamma(\sqrt{u}) - \Delta u.$$

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Li-Yau estimate:

$$(-\Delta \log u =) \qquad \frac{\Gamma(u)}{u^2} - \frac{\Delta u}{u} \leq \frac{n}{2t}.$$

but...

Identity suggests: Right thing for graphs is

$$\left(\frac{-2\sqrt{u}\Delta\sqrt{u}}{u} =\right) \qquad \frac{2\Gamma(\sqrt{u}) - \Delta u}{u} \leq \frac{n}{2t}$$

Keeping up with the curve

Goal: 'Non-negative curvature' implies:

$$\frac{2\Gamma(\sqrt{u}) - \Delta u}{u} \leq \frac{n}{t}.$$

- $CD(n, 0)$ seems not enough.

Can only prove:

Theorem

If G satisfies $CD(n, 0)$ and u is a positive solution to the heat equation on G

$$\frac{\Gamma(\sqrt{u}) - \Delta u}{u^{1-\epsilon}||u||_\infty^\epsilon} \leq O(t^{-1/2^{\epsilon^{-1}}})$$

Doesn't scale properly!!

Not strong enough to imply Harnack inequality!

Keeping up with the curve

Goal: ‘Non-negative curvature’ implies:

$$\frac{2\Gamma(\sqrt{u}) - \Delta u}{u} \leq \frac{n}{t}.$$

- $CD(n, 0)$ seems not enough.
- Problem: Lack of chain rule

CD(n,0) not enough

Recall: G satisfies $CD(n,-K)$ if for all functions $u : V(G) \to \mathbb{R}$:

$$\Gamma_2(u) = \frac{1}{2}\left[\Delta\Gamma(u) - 2\Gamma(u,\Delta u)\right] \geq \frac{1}{n}(\Delta u)^2 - K\Gamma(u)$$

Say G satisfies the *exponential curvature dimension inequality* $CDE(n,-K)$ if for all positive functions $u : V(G) \to \mathbb{R}$

$$\tilde{\Gamma}_2(u) = \frac{1}{2}\left[\Delta\Gamma(u) - 2\Gamma\left(u, \frac{\Delta u^2}{u}\right)\right] \geq \frac{1}{n}(\Delta u)^2 - K\Gamma(u)$$

at all points x such that $(\Delta u)(x) \leq 0$.

CD(n,0) not enough

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- CDE: Looks like an odd condition. In the manifold setting (and for *diffusion semigroups*) $CD(n,-K) \Rightarrow CDE(n,-K)$
- Continuous case: $CD(n,-K)$ is *equivalent* to CDE'(n,-K):

$$\tilde{\Gamma}_2(u) \geq \frac{1}{n}u^2(\Delta \log u)^2 - K\Gamma(u)$$

Exponential curvature dimension

G satisfies

- $CDE(n, -K)$ if for all positive functions $u : V(G) \to \mathbb{R}$

$$\tilde{\Gamma}_2(u) = \frac{1}{2}\left[\Delta\Gamma(u) - 2\Gamma\left(u, \frac{\Delta u^2}{u}\right)\right] \geq \frac{1}{n}(\Delta u)^2 - K\Gamma(u)$$

  at all points x such that $(\Delta u)(x) \leq 0$.

- $CDE'(n, -K)$ if for all positive functions $u : V(G) \to \mathbb{R}$

$$\tilde{\Gamma}_2(u) \geq \frac{1}{n}(\Delta \log u)^2 - K\Gamma(u)$$

Remarks:

- Exponential: CDE inequalities for u follow from CD inequality for $\log u$.
- Manifold case: $CD(n, -K)$ *equivalent* to $CDE'(n, -K)$ – but using CDE' leads to *worse* gradient estimate on graphs.

Exponential curvature dimension

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- $CDE'(n, -K)$ if for all positive functions $u : V(G) \to \mathbb{R}$

$$\tilde{\Gamma}_2(u) \geq \frac{1}{n}(\Delta \log u)^2 - K\Gamma(u)$$

What graphs satisfy these inequalities?
One example: Ricci-flat graphs of Chung and Yau (including lattices/abelian Cayley graphs)

Ricci-flat theorem

Theorem

d-regular 'Ricci-flat graphs' in sense of Chung and Yau (including $\mathbb{Z}_{d/2}$) satisfy

- $CDE(d, 0)$
- $CDE'(2.265d, 0)$

Remark: Get optimal constants (though 2.265 approximate).

Ricci-flat theorem

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- $CDE(d, 0)$
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Remark: Get optimal constants (though 2.265 approximate).

Funny fact:

- Discrete case: Necessarily lose a dimension constant by going through CDE' for $\mathbb{Z}_d$

Comparing Curvature Dimension Inequalities

Remark:

- All graphs satisfy $CD(2, -1)$
- d-regular trees don't satisfy $CDE'(n, -K)$ for *any* K!
  - A weakness of CDE'!
- Graphs of maximum degree D satisfy $CDE(2, -\frac{D}{2})$.
  - D-regular trees require curvature lower bounds like $-\frac{D}{2}$.
  - Natural, but unusual: Most graph curvature notions have fixed lower bounds that all graphs satisfy.

Recap!

Goal: Prove analogue of Li-Yau gradient estimate for positive solutions to the heat equation on non-negatively manifolds:

$$\frac{|\nabla u|^2}{u^2} - \frac{\Delta u}{u} \leq \frac{n}{2t}.$$

- Many important applications in geometry including Harnack inequalities relating maximum and minimum of solution.
- For graphs, distribution of continuous time random walk are solutions to heat equation.

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Goal: Prove analogue of Li-Yau gradient estimate for positive solutions to the heat equation on non-negatively manifolds:

$$\frac{|\nabla u|^2}{u^2} - \frac{\Delta u}{u} \le \frac{n}{2t}.$$

Needed: Notion of curvature for graphs.

- Bakry-Emery curvature dimension inequality $CD(n, -K)$ not enough
- Introduced new exponential curvature dimension inequality $CDE(n, -K)$ – weaker in manifold case.

Recap!

Goal: Prove analogue of Li-Yau gradient estimate for positive solutions to the heat equation on non-negatively manifolds:

$$\frac{|\nabla u|^2}{u^2} - \frac{\Delta u}{u} \leq \frac{n}{2t}.$$

Needed: Notion of curvature for graphs.
Needed: Replacement for logarithm

- Vital identity for Li-Yau for $f = \log u$

$$\Delta f = -\frac{|\nabla u|^2}{u^2} + \frac{\Delta u}{u} = -|\nabla f|^2 + f_t$$

- Make use of

$$2\sqrt{u}\Delta\sqrt{u} = -2\Gamma(\sqrt{u}) + \Delta u = -2\Gamma(\sqrt{u}) + u_t$$

A Theorem!

Theorem

If G satisfies $CDE(n, 0)$ and u is a positive solution to the heat equation on G

$$\frac{\Gamma(\sqrt{u})}{u} - \frac{\Delta u}{2u} \leq \frac{n}{2t}.$$

Remark:

- Direct analogue to Li-Yau inequality

$$\frac{|\nabla u|^2}{u^2} - \frac{\Delta u}{u} \leq \frac{n}{2t}.$$

A Theorem!

Gradient estimate strong enough to prove Harnack inequality?
YES!

Theorem

Suppose G satisfies the gradient estimate

$$\frac{\Gamma(\sqrt{u})}{u} - \frac{\Delta u}{u} \leq \frac{n}{2t}.$$

for u a positive function. Then for $T_1 \leq T_2$ and $x, y \in V(G)$

$$u(x, T_1) \leq u(y, T_2) \left(\frac{T_2}{T_1}\right)^{2n} \cdot \exp\left(\frac{dist(x,y)^2 \times (\max \deg(v))}{T_2 - T_1}\right)$$

Recall:

Cheeger's Inequality

If we define

$$\Phi(G) = \min_{S \subseteq G} \frac{e(S, \bar{S})}{\min\{\sum_{v \in S} \deg(v), \sum_{v \notin S} \deg(v)\}},$$

to be the conductance of a graph, then

$$\frac{\Phi(G)^2}{2} \leq \lambda_1 \leq 2\Phi(G)$$

In manifold case:

- Cheeger: $\lambda_1 \geq \frac{\Phi(G)^2}{2}$.
- Buser: $\lambda_1 = O(\Phi^2(G))$ if M has non-negative curvature.

Application

Gradient estimate + observation of Ledoux imply:

Theorem (Buser's inequality for graphs)

If G satisfies CDE(n,0) (and hence the gradient estimate)

$$\lambda_1(G) \leq C_n \Phi(G)^2$$

Gradient estimate yields Buser's inequality

Klartag, Kozma: Buser's inequality holds for graphs satisfying $CD(d, 0)$.

More applications

Gradient Estimate yields:

- Heat Kernel estimates
- Polynomial volume growth in graphs satisfying $CDE(n, 0)$

Nice theme: local graph property implies global graph property.

But wait, there's more!

Stated results for finite graphs, and non-negative curvature, but...

Have results for:

- Graphs satisfying $CDE(d, -K)$ (graphs with curvature $\geq -K$).
- Infinite graphs
- Solutions on a ball (instead of the entire graph)
- Solutions to more general Schrödinger operators: $(\Delta - \frac{d}{dt} - q)u = 0$ where $q = q(x, t)$
- ...

These imply various version of

- Harnack inequalities
- Buser's inequality
  (with curvature - of form $\lambda_1 \geq C\Phi^2 + C_2 K\Phi$)
- ...

Final remarks

Special case: Solutions to the heat equation on ‘balls’.

- Li-Yau: u solution on ball of radius R, non-negatively curved manifold.

$$\frac{|\Delta u|^2}{u^2} - \frac{\Delta u}{u} \leq \frac{n}{2t} + \frac{C}{R^2}$$

- Key: Existence of cut-off functions.
- Graph case: Cutoff function based on graph distance? Only can prove estimates of form

$$\frac{2\Gamma(\sqrt{u}) - \Delta u}{u} \leq \frac{n}{2t} + \frac{C}{R}.$$

- Can show

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if special cutoff functions exist. Can prove their existence for $\mathbb{Z}^d$. In general?

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CDE': Weaker dimension, but more powerful!

Even though $CDE'(n,0)$ required *weaker* dimension constants, it many ways it has proven to be more powerful.
In later work with Lin, Shangdong, and Yau shown $CDE'(n,0)$

- Hamilton-type gradient estimates: Gradient estimates in space (no $\frac{\partial}{\partial t}$ term)
- Showed $CDE'(n,0)$ implies 'volume doubling' (a strengthening of polynomial volume growth), and Poincaré type inequalities, sidestepping the '$\frac{1}{R}$' vs '$\frac{1}{R^2}$' problem.
- Proven diameter bounds from $CDE'(n,K)$ if $K > 0$.
- Proven heat kernel analogue of Perelman entropy formula (implying log-Sobolev type inequalities)
- $\cdots$

Method: Semigroup arguments instead of maximum principle arguments

Conclusión

Geometric methods give powerful tools and ideas to understand graphs.

Graph curvature notions give a local way to certify global geometric information.
Despite recent advances still much to understand.

Gracias!

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Geometric methods give powerful tools and ideas to understand graphs.

Graph curvature notions give a local way to certify global geometric information.
Despite recent advances still much to understand.

Gracias!