The Li-Yau Inequality and the Geometry of Graphs

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December 11, 2014
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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What to study: distribution of random walk over time.
Understanding random walks:

Behavior of random walk: Governed by shape of graph.
Understanding random walks:

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:

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

- 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
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: 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 $x \in M$

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

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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Integrating gradient estimates: Proves Harnack inequality.

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

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Li-Yau Inequality on Graphs
Bakry-Emery gradient operators:
For functions $f, g : V(G) \rightarrow \mathbb{R}$

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

Key property: In continuous case

$$\Delta(fg) = f\Delta g + g\Delta f + 2\langle \nabla f, \nabla g \rangle$$
Bakry-Emery gradient operators:
For functions $f, g : V(G) \rightarrow \mathbb{R}$

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

$$\Gamma(f, g)(x) = \frac{1}{2} (\Delta(fg) - f\Delta g - g\Delta f)$$

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

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

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

$$\Gamma_2(f) = \frac{1}{2} (\Delta \Gamma(f) - 2\Gamma(f, \Delta f))$$
An $n$-dimensional manifold $M$ with curvature $\geq -K$ satisfies the Bochner Formula

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

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

at every point $x$. 
Graph curvature

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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 its definition of curvature in many settings.
Graph curvature

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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 $f$. 
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:

\[
\Delta H \leq 0 \quad \frac{\partial}{\partial t} H \geq 0 \quad \nabla H = 0
\]

- **Discrete:** No reasonable definition of $\nabla$ 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!

\[
\Delta (\log u)(x) = \frac{1}{d_x} \sum_{y \sim x} \log \left( \frac{y}{x} \right) = ???
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  \Delta (\log u)(x) = \frac{1}{d_x} \sum_{y \sim x} \log \left( \frac{y}{x} \right) = ???
  \]
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 $p = \frac{1}{2}$:

$$-2\sqrt{u}\Delta \sqrt{u} = 2\Gamma(\sqrt{u}) - \Delta u.$$
What can replace $\Delta(\log u) = -|\nabla \log u| + \frac{\Delta u}{u}$?

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

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

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

**Li-Yau estimate:**

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

*but...*

Identity suggests: Right thing for graphs is

\[-2\sqrt{u\Delta \sqrt{u}} = \frac{2\Gamma(\sqrt{u}) - \Delta u}{u} \leq \frac{n}{2t}.\]
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!
Goal: ‘Non-negative curvature’ implies:

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

- \textit{CD}(n, 0) seems not enough.
- \textbf{Problem:} Lack of chain rule
Rethinking curvature

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 $(\Delta u)(x) \leq 0$. 

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CD(n,0) not enough

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

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

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

$G$ satisfies

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

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

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

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).
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).

**Funny fact:**

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

$$\left(\frac{\nabla u}{u^2}\right)^2 - \frac{\Delta u}{u} \leq \frac{n}{2t}.$$

- 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.
Recap!

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

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

**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

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

\[
\frac{|\nabla u|^2}{u^2} - \frac{\Delta u}{u} \leq \frac{n}{2t}.
\]
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 $x, y \in V(G)$

$$
u(x, T_1) \leq u(y, T_2) \left( \frac{T_2}{T_1} \right)^{2n} \cdot \exp \left( \frac{\text{dist}(x, y)^2 \times (\max \deg(v))}{T_2 - T_1} \right)
$$
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.
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
  \[ (\text{with curvature - of form } \lambda_1 \geq C\Phi^2 + C_2 K\Phi) \]
- ...

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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

\[
\frac{2\Gamma(\sqrt{u}) - \Delta u}{u} \leq \frac{n}{2t} + \frac{C}{R^2}
\]

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

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

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

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

Method: Semigroup arguments instead of maximum principle arguments
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.

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