The Geometry of Graphs

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Graphs

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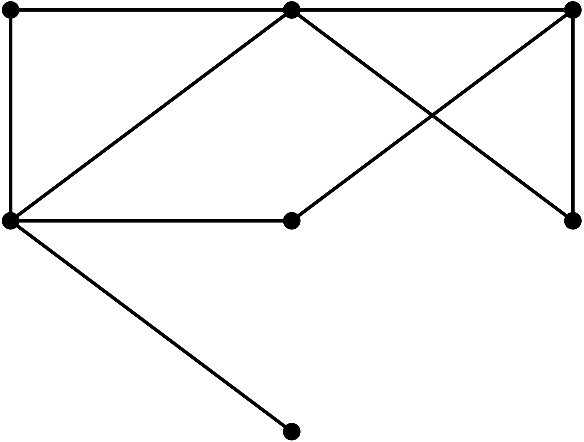
Collections of vertices and edges.



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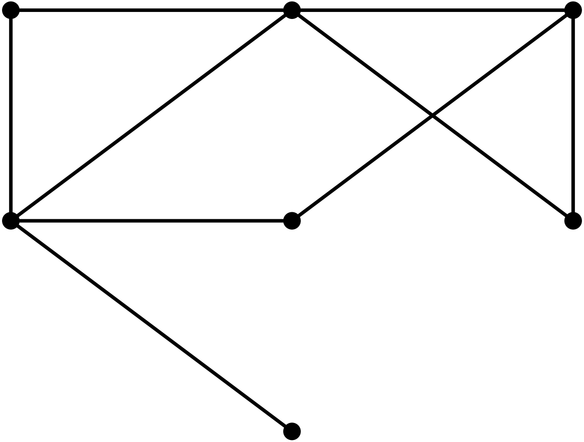

Small graph: Easy to see what's going on.

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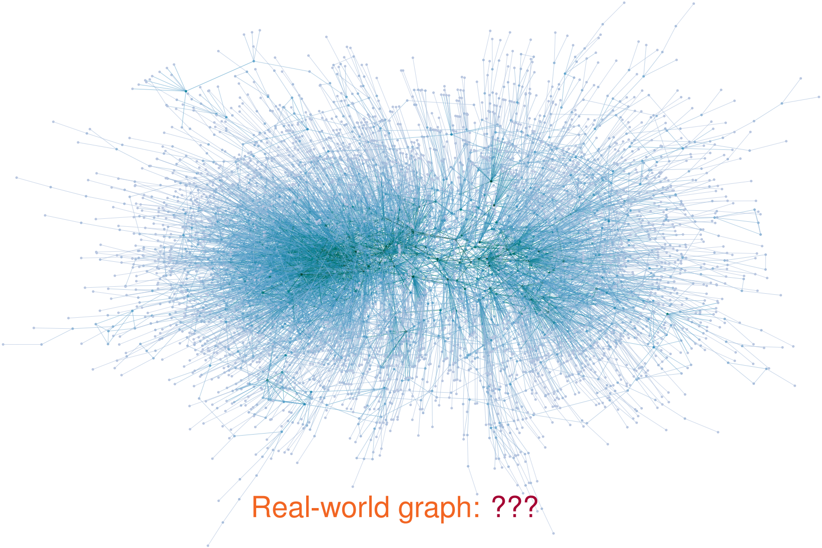

Real-world graph: ???

Challenge

Understanding large graphs leads to many challenges, especially as determining many graph properties are computationally hard.

Goals:

- Be able to *certify* graph properties ‘cheaply’ computationally.
- Understand large-scale geometric properties of graphs (diameter, cuts, etc.)

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One approach: via spectral graph theory.

Spectral Graph Theory:

Idea: Associate a matrix with a graph

Matrix eigenvalues $\Leftrightarrow$ Graph properties

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- Unsymmetrized version of $-\mathcal{L} = D^{-1/2}AD^{-1/2} - I$
  (normalized Laplacian ala Chung)
- Eigenvalues: $0 = -\lambda_0 \leq -\lambda_1 \leq \cdots \leq -\lambda_{n-1} \leq 2$.
- $-\lambda_1 > 0 \iff G$ connected
  $(\#0's = \#$ connected components$)$
  $-\lambda_{n-1} < 2 \iff$ no bipartite component.

Geometry and Eigenvalues

Cheeger's Inequality

If G is a graph, and λ_1 is the absolute value of second eigenvalue of Δ, then

$$2\Phi \geq \lambda_1 \geq \frac{\Phi^2}{2}$$

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

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- Quantitative version of statement that $\#0's = \#$ cc.
- Bound $\lambda_1 \geq \frac{\Phi^2}{2}$: exact analogue of Cheeger's inequality from differential geometry.
- Bound $2\Phi \geq \lambda_1$: trivial for graphs, and not part of Cheeger's inequality in geometry.

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- Bound $\lambda_1 \geq \frac{\Phi^2}{2}$: exact analogue of Cheeger's inequality from differential geometry.
- Bound $2\Phi \geq \lambda_1$: trivial for graphs, and not part of Cheeger's inequality in geometry.
- Buser's inequality: Non-negatively curved manifolds satisfy $\lambda_1 = O(\Phi^2)$.

Spectral Graph Theory

Graph eigenvalues control many geometric properties of graphs:

- Isoperimetric constant (via Cheeger's inequality)
- Diameter/distance between subsets
- Diffusion of random walks/heat dispersion.
- ...

Eigenvalues provide a certificate of many graph properties, but are *global* in nature.

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Goal: Find local way to certify similar geometric properties.

Curvature on Graphs

- Curvature of manifold: *Local* quantity measuring how fast manifold expands near a point
  - Zero curvature: (Locally) expands like $\mathbb{R}^n$
  - Positive curvature: (Locally) expands slower than $\mathbb{R}^n$ (like on sphere)
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- Curvature lower bounds have strong geometric and analytic consequences.
  - eg. Bochner Formula: If M is an n-dim'l manifold, curvature $\geq -K$, then for all smooth $f : M \to \mathbb{R}$

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

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- Definitions of curvature for graphs take a consequences and make it a *definition* in the graph case. eg. based on:
  - Degree (natural measure of local expansion)
  - 'Transportation distance' (Ollivier/Lott, Villani/Lin, Lu, Yau)
  - Satisfying analytic condition like Bochner Formula.

Road to understanding

One major route to understanding geometric properties from curvature:

Curvature lower bound

$\Downarrow$

Control of solutions to heat equation

(solns to $\frac{\partial}{\partial t} u = \Delta u$)

$\Downarrow$

Geometric information on graph/manifold

Road to understanding

One major route to understanding geometric properties from curvature:

$$\begin{gathered}\text{Curvature lower bound} \\ \Downarrow \\ \text{Control of solutions to heat equation} \\ (\text{solns to } \tfrac{\partial}{\partial t}u = \Delta u) \\ \Downarrow \\ \text{Geometric information on graph/manifold}\end{gathered}$$

Grigor'yan and Saloff-Coste (for manifolds) and Delmotte (for graphs) show:

- Strong control of solutions (Harnack inequalities) $\Leftrightarrow$
- Eigenvalue condition on balls (Poincaré inequality) plus volume growth condition (volume doubling) $\Leftrightarrow$
- Gaussian behavior for fundamental solutions.

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Geometric information on graph/manifold

- Manifold case: A curvature lower bound implies the Li-Yau inequality, a local estimate of how heat diffuses.
- Li-Yau Inequality: If u positive solution to heat equation on n-dim'l non-negatively curved compact manifold,

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

- Can be integrated to derive Harnack inequality, and imply three (equivalent) conditions.

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Geometric information on graph/manifold

- Version of Li-Yau inequality for graphs derived by Bauer, H., Lippner, Lin, Mangoubi, Yau
- Introduce new version of graph curvature, the exponential curvature dimension inequality
- Can derive a Harnack inequality, but not quite strong enough to imply three conditions.
- H., Lin, Liu, Yau: Use different methods to prove non-negatively curved graphs satisfy equivalent conditions.

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Geometric information on graph/manifold

Remark: Understanding solutions to the heat equation themselves is interesting on graphs. Related to diffusion of continuous time random walk.

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Geometric information on graph/manifold

To continue, want to revisit

Key step: Proving Li-Yau inequality for graphs.

Goal

To prove Li-Yau inequality for graphs, and its further geometric consequences need to understand how curvature plays a role in the proofs.

Challenges that arise dictate how to proceed.

Li-Yau proof:

To understand Li-Yau inequality for graphs, need to understand proof of inequality for manifold. For original proof

Key ideas:

- Bound function $H(x,t) = t\left(\frac{|\nabla u|^2}{u^2} - \frac{u_t}{u}\right)$. Use maximum principle. At max. pt:

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

- Get inequality relating H and H^2 by applying Bochner formula and key identity (from chain rule):

$$(-H/t) = \Delta \log u = -|\nabla \log u|^2 + (\log u)_t$$

- Curvature enters through Bochner formula

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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Observed: Bochner formula only real application of curvature in proof

From work of Bakry, Emery: Can be used as it definition of curvature in many settings.

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

Bakry-Emery gradient operators:

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

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

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

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at every point x.

Curvature-Dimension Inequality

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

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

for every function f.

Curve ball

- Every graph satisfies $CD(2, -1 + \frac{1}{\max \deg(v)})$.

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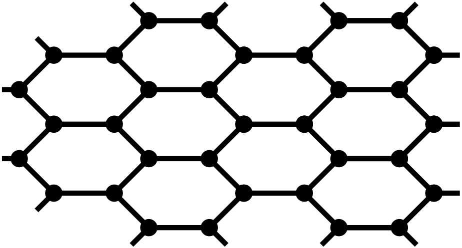

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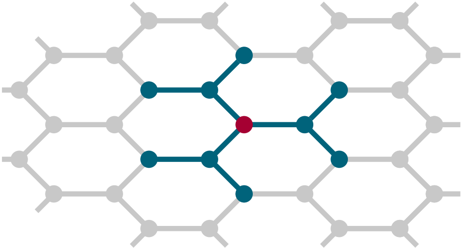

Feature/Drawback: Truly local, doesn't capture beyond 2nd neighborhood.

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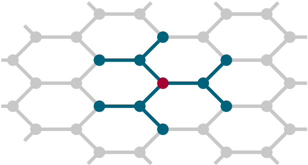

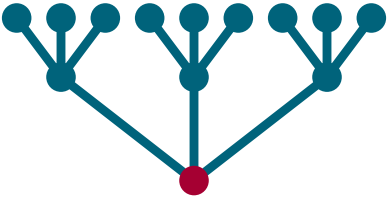

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Bochner formula: Key to proof of Li-Yau inequality. $CD(n, 0)$ enough in graph case?

Chain rule:

Key identity: In manifold case, the fact that

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

is key, but is false for graphs as Δ does not satisfy the chain rule.

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Infinite family of identities: On manifolds

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

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

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

Rethinking curvature

$CD(n, 0)$ not enough

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

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

Even with the identity $-2\sqrt{u}\Delta\sqrt{u} = 2\Gamma(\sqrt{u}) - \Delta u$ in hand, $CD(n, 0)$ is insufficient – again because of terms that do not vanish because of the chain rule.

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Exponential curvature dimension

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

REDACTED: UGLY FUNCTIONAL INEQUALITY

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

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- CDE: Looks like an odd condition. But, in manifold setting: $CD(n, -K) \Rightarrow CDE(n, -K)$
- Continuous case: $CD(n, -K)$ is *equivalent* to slight variant $CDE'(n, -K)$.

G satisfies

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

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Exponential curvature dimension

G satisfies

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

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

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

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

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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 *weaker* dimension constants in graph case.
- H., Lin, Liu, Yau: G satisfying $CDE'(n, 0)$ allows one to derive much more than Li-Yau

Exponential curvature dimension

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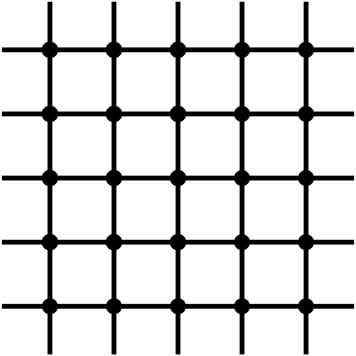
What graphs satisfy these inequalities?
One example: Ricci-flat graphs of Chung and Yau

Ricci-flat graphs

What are Ricci-flat graphs



Key Lattice property: Move a direction, look at neighborhood same as look at neighborhood, and move a direction.

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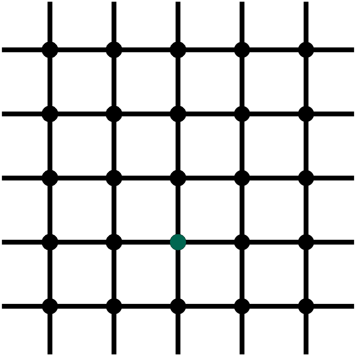

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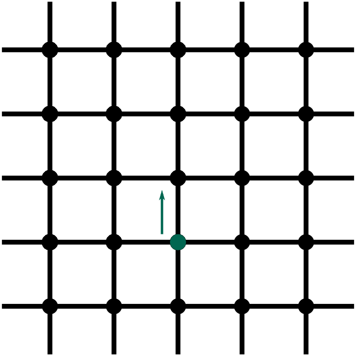

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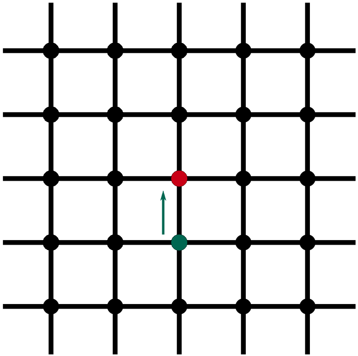

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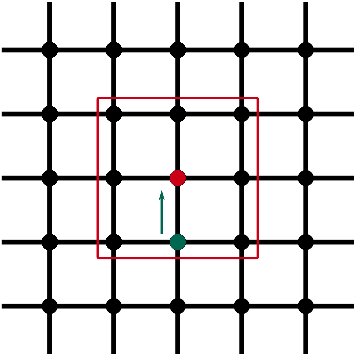

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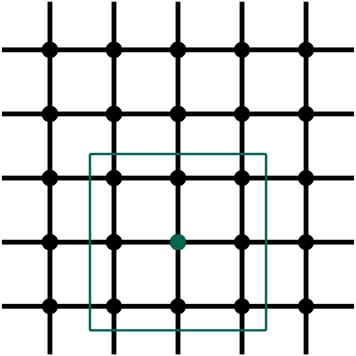

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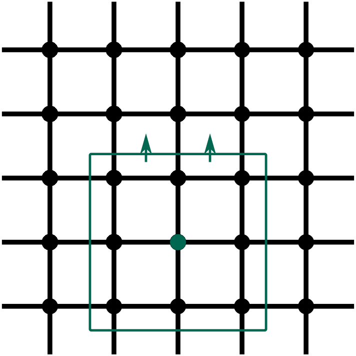

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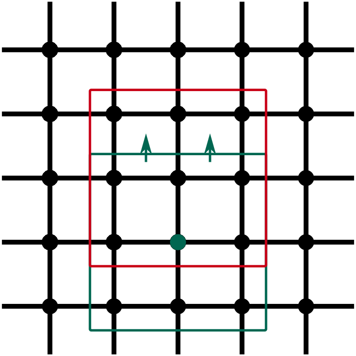

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Ricci-flat theorem

Theorem (Bauer, H., Lin, Lippner, Mangoubi, Yau)

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: We get the optimal constants.

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 $CD(2, -1)$
- Graphs of maximum degree D satisfy $CDE(2, -\frac{D}{2})$.
  - D-regular trees require curvature lower bounds like $-\frac{D}{2}$.
  - Unusual but natural: Most graph curvature notions have fixed lower bounds that all graphs satisfy.

Li-Yau

Theorem (Bauer, H., Lin, Lippner, Mangoubi, Yau)

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

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

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Remark:

- Direct analogue to Li-Yau inequality

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

- Form follows from key identity $-2\sqrt{u}\Delta\sqrt{u} = 2\Gamma(\sqrt{u}) - \Delta u$.

Li-Yau

Gradient estimate strong enough to prove Harnack inequality.

Theorem (Bauer, H., Lin, Lippner, Mangoubi, Yau)

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 $x, y \in V(G)$

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

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 $CD(d, 0)$.

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- Further can prove: Graphs which are positively curved satisfying $\lambda_1 \geq \frac{C}{\mathrm{diam}(G)^2}$ for positively curved graphs (in terms of CDE).

Beyond Li-Yau

Despite its applications, our Li-Yau inequality is not quite strong enough for some applications:

- Harnack inequality not strong enough to imply volume doubling/Poincaré and Gaussian bounds.
- One reason: Distance function not controlled enough for cutoff functions
- Another: *CDE* only gives control at points where $\Delta u \leq 0$ – makes global arguments difficult.
- Second point: rules out approaches based on heat semigroup.

H., Lin, Liu, Yau: Use CDE’ to run semigroup arguments to prove stronger conclusion.

Curvature implies volume doubling/Poincaré and Gaussian bounds

H., Lin, Liu, Yau:

- Adapt variational inequality of Baudoin and Garofalo to graph setting.

Further prove:

- (Family of) Li-Yau type inequalities for graphs satisfying $CDE'(n, 0)$
- $CDE'(n, 0)$ implies:
  - Volume doubling/Poincaré inequality
  - Gaussian bounds for discrete time random walk
  - (Stronger) Harnack inequality.
- Bonnet-Myers theorem for positively curved graphs (get explicit diameter bound)

Key idea: By switching to more global arguments (enabled by CDE'!), we avoid problems encountered in our previous work on using graph distance to define cutoff functions.

Curvature to volume doubling/Poincaré

Ultimately: we would like to prove directly that we satisfy one of the three equivalent conditions of Delmotte:

- Harnack inequality (of proper form)
- Volume Doubling + Poincaré inequality
- Gaussian bounds for (discrete) solutions to the heat equation

If we had one of these conditions directly, we'd be done. Unfortunately we don't quite do any of this directly. Proof comes from establishing (slightly weaker) Harnack inequality (akin to our previous work) plus volume doubling, and using this to imply Gaussian bounds in a hybrid way (similar to, but not quite the same as the arguments of Delmotte).

Fin

- Curvature of graphs is a powerful way of controlling global graph properties from local information.
- CDE and CDE' inequalities 'bake in the chain rule' and allow us to derive strong results about the structure of graphs.
- BHLLMY: Li-Yau inequality and applications from CDE.
- HLLY: Volume doubling/Poincaré and Gaussian bounds, along with Bonnet-Myers type theorems from CDE'.
- Beyond (H, BH): Eigenvalue inequalities, Hamilton type gradient estimates...
- Still a lot to come.

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Thank You!