A SPACIAL GRADIENT ESTIMATE FOR SOLUTIONS TO THE HEAT EQUATION ON GRAPHS*

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Abstract. The study of positive solutions of the heat equation $\frac{\partial}{\partial t}u = \Delta u$, on both manifolds and graphs, gives an analytic way of extracting geometric information about the object. In the manifold case, one of the most effective ways of studying how solutions to the heat equation evolve is to derive a local 'gradient estimate' of heat change, using curvature lower bounds. Recently, notions of curvature for graphs have been developed which enable proving similar estimates for graphs. In this article, we derive a gradient estimate for positive heat solutions that considers only how heat varies in space and the time derivative. This result, due in the manifold case to Hamilton, applies to both finite graphs and infinite graphs of bounded degree. As a corollary, a heat comparison theorem is also developed. This in turn yields results about the mixing of the continuous time random walk on graphs.

Key words. heat equation, gradient estimate, curvature, curvature dimension inequality, continuous time random walk

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The study of positive solutions to the heat equation, $\frac{\partial}{\partial t}u = \Delta u$, is of fundamental importance in Riemannian geometry and geometric analysis. This is, in large part, because the evolution of solutions on manifolds is closely related to the underlying geometric properties of the manifolds. Indeed, as shown (independently) by Grigor'yan [8] and Saloff-Coste [17], Gaussian decay of the heat kernel is *equivalent* to satisfying a Poincaré inequality (an eigenvalue inequality) and volume doubling (a statement about the growth of balls), and in turn is also equivalent to solutions satisfying a strong Harnack inequality, allowing comparison of 'heat' at different points at different times.

In a graph setting, studying solutions to the heat equation makes sense for a broad class of Laplace operators Δ. For the purposes of this discussion, consider $\Delta = D^{-1}A - I$ which is an unsymmetrized version of the *normalized Laplacian* popularized by Chung (see [3].) Here, solutions of the heat equation have a particularly nice probabilistic interpretation: they reflect the evolution of the so-called continuous time random walk where a random walker stays on a vertex for an exponentially distributed amount of time. In the graph setting, equivalence of the three properties (Gaussian decay of the heat kernel, Poincaré plus volume doubling, and strong Harnack inequality) is also known, due to work of Delmotte in [7]. These reflect the fact that the evolution of the continuous time random walk is closely related to geometric properties of the graph (eg. volume doubling, diameter bounds, etc.) Studying this evolution gives an analytic way of understanding geometric properties of a graph.

One question remains: how to show that a graph *satisfies* one, and hence all, of these three equivalent conditions in an 'easy' fashion. In the Riemannian setting, a curvature lower bound provides an easy way to do exactly that through the Li-Yau inequality, derived in [12]. This inequality bounds the local change of heat in space and time. Curvature lower bounds (with an appropriate notion of curvature) are an appealing way to establish properties of graphs as curvature is a 'local' property and many of the implications of a curvature bound are 'global.' Thus, using 'curvature' to

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understand properties of a graph involves understanding global geometric properties of large graphs by understanding the 'local behavior' – ie. it studies how one can understand global properties of a graph by looking only at behavior of vertices and neighbors to some (bounded) distance. Curvature also often give a uniform way of establishing results on both finite and infinite graphs.

In the graph setting, only recently have curvature notions been introduced which are strong enough to show that a graph satisfies these equivalent properties. In [2], Bauer, Lin, Lippner, Mangoubi, Yau and the author a version of the Li-Yau inequality for graphs as proved. While it not quite strong enough to 'complete the cycle' and prove that non-negative curvature implies the three equivalent conditions, was able to establish that non-negatively curved graphs had polynomial volume growth among other properties. Later work of the author, Lin, Liu and Yau [10] used a slight variant of the curvature condition of [2] and some different arguments to establish not only the three equivalent conditions, but also to establish from non-negative or positive curvature a number of geometric properties of graphs, such as diameter and volume bounds.

In this note, we further our study of the heat equation. The Li-Yau inequality of [12] (in its simplest form, for compact n-dimensional manifolds which are non-negatively curved) states that a positive solution to the heat equation satisfies

$$\frac{|\nabla u|^2}{u^2} - \frac{u_t}{u} \leq \frac{n}{2t}. \tag{1}$$

This inequality relates how the solution changes in space ($|\nabla u|$) and also in time (u_t) in a way that decays as time increases. To derive a Harnack inequality, which compares the heat of two points at two different times, one takes a path in spacetime between the two points and carefully integrates the inequality to see how the heat can change.

One interesting aspect to this is that (1) requires the $-\frac{u_t}{u}$ term to make sense: the quantity $\frac{|\nabla u|^2}{u^2}$ is not able to be bounded by an absolute constant. The net effect of this is that the Li-Yau inequality cannot be integrated to compare the heat of two points at the same time. Nonetheless, Hamilton [9] showed that the heat 'almost' behaves well in time, proving that the if u is a solution to the heat equation, normalized so that $||u||_\infty = 1$, for a compact n-dimensional non-negatively curved manifold, then

$$\frac{|\nabla u|^2}{u^2} \leq \frac{1}{t} \log(1/u). \tag{2}$$

Note that the normalization $||u||_\infty = 1$ appearing is in a sense required as the inequality is not invariant to normalization (unlike the original Li-Yau inequality and the Li-Yau inequality for graphs proved in [2].)

Our main purpose of this note is to derive a version of Hamilton's Li-Yau inequality, (2), for graphs. Like Hamilton's version, our inequality is dimension independent: this is particularly interesting as this allows us to apply our work to certain *directed* graphs, which are in a sense 'infinite dimensional' flat graphs. We go somewhat beyond the work of Hamilton by providing a version of our inequality which applies to infinite graphs as well – the original work of Hamilton only considers the compact manifold case which translates to finite graphs.

In the next section we give some preliminary notation and information on the curvature notions used. In Section 3 we prove our main results. Finally, we prove a heat comparison theorem, in the vein of a Harnack inequality, and give some applications and discussion in Section 4.

1. Background and Notation. Let $G = (V, E)$ be a locally finite graph with maximum degree D, infinite or finite. Our graph theory notation is quite standard throughout: we use $x \sim y$ to denote that vertex x is a neighbor of y, $d(x, y)$ to denote the distance between x and y in the standard graph metric, and $\mathrm{diam}(G)$ to denote the diameter of G (for finite graphs).

We assume edges are weighted with weights $w_{xy} > 0$, and make the further assumption that

$$w_{min} = \inf_{xy \in E} w_{xy} > 0.$$

We don't assume a priori that the edge weights are symmetric. As a convention, we assign the edge weight w_{xy} to the edge from x to y. Most (but not all) of the graphs known to be 'flat' with respect to the curvature conditions below are undirected, however there do exist some weighted 'flat' graphs and our methods do apply to them.

Let $\mu : V \to \mathbb{R}^+$ be a positive measure on the vertices with $\inf_{x \in V} \mu(x) = \mu_{min} > 0$. The μ-Laplace operator on the graph is the following operator: If $f : V \to \mathbb{R}$ is a

$$(\Delta f)(x) = \frac{1}{\mu(x)} \sum_{y \sim x} w_{xy}(f(y) - f(x)).$$

While μ may be chosen to be an arbitrary measure, the most classical choices of μ are $\mu \equiv 1$ (which leads to the combinatorial Laplace operator) and $\mu(x) = \deg(x) = \sum_{y \sim x} w_{xy}$ which leads to the *normalized* Laplace operator. While our methods apply to arbitrary Laplace operators, the reader is quite welcome to think of the results in terms of these classical cases. In the case of finite graphs, these *almost* agree with the classical combinatorial Laplacian matrix $D - A$ and the normalized Laplacian $I - D^{-1/2}AD^{-1/2}$. The sign convention is changed to agree with the Laplace-Beltrami operator on manifolds (the operator is non-positive semidefinite as opposed to the matrices which are positive semidefinite) and the normalized Laplacian $I - D^{-1/2}AD^{-1/2}$ of Chung is a symmetrized version of this operator.

In general, our results are agnostic to the measure μ, and we use the notation $\widetilde{\sum}$ to denote the types of averaged sum appearing in (1). That is, for real numbers a_x we let

$$\widetilde{\sum_{y \sim x}} x_y := \frac{1}{\mu(x)} \sum_{y \sim x} w_{xy} x_y.$$

As a convenience we record here some assumptions and notational convetions, we use regarding the measures involved.

ASSUMPTIONS: *Our measures $\mu : V \to \mathbb{R}^+$ and edge weights w_{xy} satisfy*

$$w_{min} = \inf_{xy \in E} w_{xy} > 0, \tag{3}$$

$$\mu_{\min} = \inf_{x \in V} \mu(x) > 0, \tag{4}$$

$$D_{\max} = \sup_x \frac{\deg(x)}{\mu(x)} = \sup_x \frac{1}{\mu(x)} \sum_{y \sim x} w_{xy} < \infty, \tag{5}$$

$$\mu_{\max} = \sup_{x \in V} \mu(x) < \infty. \tag{6}$$

As an immediate consequence of our assumptions, we record

Lemma 1. $\{a_x\}_{x\in V(G)}$ *are a positive numbers,*

$$\widetilde{\sum_{y\sim x}} a_y \leq D_{\max} \cdot \max_{y\sim x} a_y.$$

1.1. Curvature Notions on Graphs. There have been, over the past few years, a large number of curvature notions developed for graphs. These all have the feature that the 'curvature' at a vertex (or, in some cases across an edge), depend on the structure on the graph in a bounded iterated neighborhood of the vertex. Of these two have perhaps attracted the most attention recently. The first of those is based on the notion of transportation distance (see eg. papers of Lott-Villani [15], Ollivier [16], and Lin, Lu and Yau [13]), where curvature is measured by how well random walks at different points can be coupled. The other takes a more analytic tilt, and is based on the idea of a curvature dimension inequality.

The idea of curvature dimension inequalities, is to define the notion of curvature lower bounds where the may not other be defined, by via the Bochner formula The Bochner formula states that in an n-dimensional manifold M with curvature $\geq -K(n-1)$ that for all smooth functions u, the inequality

$$\frac{1}{2}\Delta|\nabla u|^2 \geq \langle \nabla u, \nabla \Delta u\rangle + \frac{1}{n}(\Delta u)^2 - K|\nabla u|^2 \tag{7}$$

holds at every point on M.

Remark: For the reader in graph theory, functional inequalities like (7) are perhaps unfamiliar. Throughout the paper, when we assert a pointwise inequality of functions, we omit the arguments unless it makes our inequality clearer. Also note that if u is a function, so are Δu and $|\nabla u|^2$ as are all the terms appearing in (7).

Bakry and Emery observed (see [1]) that on spaces where a Laplace operator Δ was defined one could define a gradient operator Γ, formally setting

$$\langle \nabla f, \nabla g\rangle = \Gamma(f,g) := \frac{1}{2}\left(\Delta(fg) - f\Delta g - g\Delta f\right).$$

For graphs, at a vertex x and for two functions $f, g : V \to \mathbb{R}$, the function $\Gamma(f,g) : V \to \mathbb{R}$ simplifies to

$$\Gamma(f,g)(x) = \widetilde{\sum_{y\sim x}}(f(y)-f(x))(g(y)-g(x)).$$

As a convenience, we let $\Gamma(f) := \Gamma(f,f)$ which serves as a replacement for $|\nabla f|^2$ in the graph setting. (Note $\Gamma(f)(x) = \widetilde{\sum}_{y\sim x}(f(y)-f(x))^2$, and in particular $\Gamma(f) \geq 0$.)

Bakry and Emery further noted that whena diffusive semigroup satisfies an analogue of Bochner formula (7) many properties implied by a curvature lower bound can be recovered. To this end, they introduced the iterated gradient form Γ_2 which is defined by

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

Then, a space with some Laplace operator Δ (eg. a graph, manifold, or diffusive semigroup) is said to satisfy the curvature dimension inequality $CD(n,-K)$ if at every point and for every (smooth in the continuous case) function f,

$$\Gamma_2(f)(x) \geq \frac{1}{n}(\Delta f)(x)^2 - K\cdot\Gamma(f)(x).$$

The intuition is that a graph satisfying $CD(n,-K)$ should behave like a n-dimensional manifold with a curvature lower bound of $-K$. While it is indeed true that some analytic consequences of non-negative curvature (for instance) can be established for graphs satisfying $CD(n,0)$ (see eg. [4, 11, 14]), the standard curvature dimension inequality on graphs has some limitations. Many applications of the Bochner formula require the Laplace operator to satisfy a chain rule. This holds in the diffusive semigroup setting considered by Bakry and Emery in [1], but fails in general for graphs. To overcome this difficulty, in [2] two alternate versions were introduced, the so called *exponential* curvature dimension inequalities, which in a sense bake in the chain rule.

Definition 2. *A graph is said to satisfy the* **exponential curvature dimension inequality** $CDE(n,-K)$ *if at every vertex x and at for every function $f : V \to \mathbb{R}^{\geq 0}$ so that* $(\Delta f)(x) \leq 0$

$$\tilde{\Gamma}_2(f) := \frac{1}{2}\Delta\Gamma(f) - \Gamma\left(f, \frac{\Gamma(f^2)}{2f}\right) \geq \frac{1}{n}(\Delta f)^2 - K\Gamma(f).$$

Definition 3. *A graph is said to satisfy the* **exponential curvature dimension inequality** $CDE'(n,-K)$ *if at every vertex x and at for every function $f : V \to \mathbb{R}^{\geq 0}$*

$$\tilde{\Gamma}_2(f) := \frac{1}{2}\Delta\Gamma(f) - \Gamma\left(f, \frac{\Gamma(f^2)}{2f}\right) \geq \frac{1}{n}f(x)^2(\Delta \log f)^2 - K\Gamma(f).$$

Remark: Observe that if G satsifies $CDE(n,-K)$ or $CDE'(n,-K)$ then it satisfies $CDE(n',-K')$ for any $n' \geq n$ and $-K' \leq -K$. Hence these inequalities weaken as the dimension increases or the curvature lower bound decreases. Our results actually apply to graphs satisfying $CDE(\infty,-K)$ for some $K \geq 0$; that is we will discard the $(\Delta f)^2$ term appearing above.

These two inequalities are closely related, and indeed it is easy to see by Jensen's inequality that if a graph satisfies $CDE'(n,-K)$ it also satisfies $CDE(n,K)$. Every graph satisfies $CDE(2,-d_{\max})$ but a number of graphs are known to be non-negatively curved with respect to these curvature notions. For instance, it is known that d-regular Ricci-flat graphs, in the sense of Chung and Yau (see [5, 6]) satisfy $CDE'(3d,0)$ and $CDE(d,0)$ by work of [2]. bIt is also known that certain *directed* Ricci-flat graphs (called in [2] Ricci-flat graphs with weakly consistent weights), where edges in different 'directions' are weighted differently also satisfy $CDE'(\infty,0)$ though they do not satisfy $CDE'(n,0)$ (nor $CDE(n,0)$) for any finite n. Quite interestingly, our results apply to these as well.

Both the CDE and CDE' inequality are also closely related to the classical CD inequality. Indeed, for diffusive semigroups (essentially, when the Laplace operator satisfies the chain rule) $CDE'(n,-K)$ and $CD(n,-K)$ are equivalent. On graphs, they are *not* equivalent. $\mathbb{Z}^d$, for instance, satisfies $CD(2d,0)$, but does not satisfy $CDE'(2d,0)$ and only satisfies the weaker inequality $CDE'(4.53d,0)$.

While BHMMLY use the CDE inequality in their work on the Li-Yau inequality, the $CDE'(n,0)$ has proven quite useful for a number of arguments. Indeed, in the work of Lin, Liu, Yau and the author establishing the strong Harnack inequality for non-negatively curved graphs $CDE'(n,0)$ is used as it allows more 'global' arguments to be used. This is due to the fact that the CDE inequality only gives an inequality at a point when $\Delta f < 0$, while the CDE' inequality asserts a non-trivial lower bound on $\tilde{\Gamma}_2$ at every point. In this work, we will use the CDE inequality as this yields slightly stronger results.

1.2. The Heat Equation on Graphs. In this paper we study positive solutions to the heat equation; that is $u : V \times [0, \infty) \to \mathbb{R}$ satisfying

$$\frac{\partial}{\partial t} u = \Delta u$$

for $t \geq 0$. As is well known, these solutions are determined by the initial values $u_0 : V \to \mathbb{R}$. For any such u_0, it is easy to see that $u = e^{t\Delta} u_0$ is a solution to the heat equation.

These solutions are closely related to a type of random walk on graphs, the so-called *continuous time random walk.* In a continuous time random walk, a simple random walk is performed where the amount of time the walker spends before taking a random step is exponentially distributed, instead of the walker spending one time step before taking a step. Indeed, if Δ is defined with $\mu(v) = \deg(v) = \sum_{u \sim v} w_{vu}$ – that is when we consider the normalized Laplace operator – the distribution, φ_t, of a continuous time random walk at time t starting at initial distribution φ_0

$$(\varphi_t)^T = (\varphi_0)^T e^{t\Delta}.$$

For a regular graph, the normalized Laplace operator is symmetric, and so the φ_t is a solution to the heat equation. For irregular graphs, one has to translate between the two but this is possible. For a finite graph and positive u, $e^{t\Delta} u$ tends to the constant function as $t \to \infty$ while $u^T e^{t\Delta}$ tends towards a vector proportional to the degrees (that is to the stationary distribution of the random walk).

2. Main Results. In this section we record and prove our main results, which are graph theoretical versions of a gradient estimate for solutions to the heat equation that is originally due to Hamilton. Unlike the original Li-Yau inequality, which controls both a combination of the gradient and time derivative of positive solutions to the heat equation, the Hamilton gradient estimate is concerned solely with the gradient – how a solution varies in time.

For convenience, we define the operator $\mathcal{L}$,

$$\mathcal{L} = \left(\Delta - \frac{\partial}{\partial t} \right).$$

As we will use the maximum principle repeatedly, we make a brief observation. Suppose $f : V \times [0, \infty) \to \mathbb{R}$ is maximized on $V \times (0, T)$ at (x^*, t^*). Then $\Delta f(x^*, t^*) \leq 0$ and $\frac{\partial}{\partial t} f(x^*, t^*) \geq 0$, so that $\mathcal{L}(f) \leq 0$. Also, we will frequently use that if $f, g : V \times [0, \infty) \to \mathbb{R}$

$$\begin{aligned} \mathcal{L}(f \cdot g) &= \Delta(f \cdot g) - \frac{\partial}{\partial t} f \cdot g = \Delta(f) \cdot g + f \cdot \Delta(g) + 2\Gamma(f, g) - f_t \cdot g - f \cdot g_t \\ &= \mathcal{L}(f) \cdot g + f \cdot \mathcal{L}(g) + 2\Gamma(f, g). \end{aligned}$$

As an initial step, we make the record the following computation (which partially motivated the definition of the definition of $\tilde{\Gamma}_2$ in [2].)

LEMMA 4. *If u is a positive solution to the heat equation $\frac{\partial}{\partial t} u = \Delta u$, then*

$$\mathcal{L}(\Gamma(\sqrt{u})) = 2\tilde{\Gamma}_2(\sqrt{u}).$$

Proof. We record that

$$\mathcal{L}(\Gamma(\sqrt{u}) = \Delta(\Gamma(\sqrt{u})) - \frac{\partial}{\partial t}\Gamma(\sqrt{u}).$$

Then at a vertex x, and time t

$$\begin{aligned}
\frac{\partial}{\partial t}\Gamma(\sqrt{u})(x,t) &= \frac{\partial}{\partial t}\frac{1}{2}\cdot \widetilde{\sum_{y\sim x}}(\sqrt{u}(y,t) - \sqrt{u}(x,t))^2 \\
&= \widetilde{\sum_{y\sim x}}(\sqrt{u}(y,t) - \sqrt{u}(x,t))\left(\frac{u_t(y,t)}{2\sqrt{u}(y,t)} - \frac{u_t(x,t)}{2\sqrt{u}(x,t)}\right) \\
&= \widetilde{\sum_{y\sim x}}(\sqrt{u}(y,t) - \sqrt{u}(x,t))\left(\frac{(\Delta u)(y,t)}{2\sqrt{u}(y,t)} - \frac{(\Delta u)(x,t)}{2\sqrt{u}(x,t)}\right) \\
&= 2\Gamma\left(\sqrt{u}, \frac{\Delta u}{2\sqrt{u}}\right)(x,t),
\end{aligned}$$

and combining gives us what we desire. □

We are ready to prove our main theorem. We prove two versions of the theorem; the first for finite graphs.

THEOREM 5. *Suppose $G = (V,E)$ is a finite graph which satisfying $CDE(\infty, -K)$ for some $K \geq 0$, and u is a positive solution to the heat equation with $||u||_\infty = 1$. Then at all $x \in V(G)$ and $t \in (0,\infty)$,*

$$\frac{\Gamma(\sqrt{u})}{u} \leq \left(\frac{1}{t} + 2K\right)\log\left(\frac{1}{u}\right).$$

Remark: A word of explanation is warranted for the form of this inequality: the original inequality of Hamilton bounded $\frac{|\nabla u|^2}{u^2} \leq \frac{1}{t}\log(\frac{1}{u})$, while we essentially bound $\frac{|\nabla\sqrt{u}|^2}{u}$ instead. This yields a slightly weaker gradient estimate, but for reasons discussed in [2] this is really necessary for small time in graphs. That we bound the gradient of the square root of u instead of the gradient of u is also tied to the chain rule and the definition of the CDE inequality.

Proof of Theorem 5. As a preliminary computation, we record that at any vertex

x, and any time t

$$
\begin{aligned}
&-\Gamma(\sqrt{u})(x,t)+\mathcal{L}(u\log(u))(x,t)\\
&\quad=-\Gamma(\sqrt{u})(x,t)+\mathcal{L}(u)\log(u)(x,t)+u\mathcal{L}(\log u)(x,t)+2\Gamma(\log(u))(x,t)\\
&\quad=-\Gamma(\sqrt{u})(x,t)+u\left(\Delta\log u-\frac{\Delta u}{u}\right)(x,t)+2\Gamma(u,\log u)(x,t)\\
&\quad=-\Gamma(\sqrt{u})(x,t)-(\Delta u)(x,t)+u(x,t)\cdot\widetilde{\sum_{y\sim x}}\big(\log(u(y,t))-\log(u(x,t))\big)\\
&\qquad\qquad+\widetilde{\sum_{y\sim x}}\big(u(y,t)-u(x,t)\big)\big(\log(u(y,t))-\log(u(x,t))\big)\\
&\quad=-\Gamma(\sqrt{u})(x,t)-(\Delta u)(x,t)+\widetilde{\sum_{y\sim x}}u(y,t)\log\left(\frac{u(y,t)}{u(x,t)}\right)\\
&\quad=\widetilde{\sum_{y\sim x}}\left[-\frac{1}{2}(\sqrt{u(y,t)}-\sqrt{u(x,t)})^2+(u(x,t)-u(y,t))-u(y,t)\log\left(\frac{u(x,t)}{u(y,t)}\right)\right] \qquad (8)\\
&\quad\geq 0.
\end{aligned}
$$

Here, in the last inequality, we use the fact that for $a,s>0$ (as we consider a positive solution to the heat equation), the function

$$f(s)=-\frac{1}{2}(\sqrt{s}-\sqrt{a})^2+(s-a)-a\log(s/a)$$

is minimized when $s=a$, at which point $f(s)=0$. Indeed, a simple calculation shows that

$$f'(s)=-\frac{(\sqrt{s}-\sqrt{a})}{2\sqrt{s}}+1-\frac{a}{s}=\frac{(\sqrt{s}-\sqrt{a})(\sqrt{s}+2\sqrt{a})}{2s}.$$

This has a single critical point at $s=a$, which clearly is the global minimum.

As each of the summands in (8) is non-negative so is the averaged sum. In fact, the inequality above is strict unless u is constant on x and all of its neighbors.

Let

$$
\begin{aligned}
H&=\frac{t}{1+2Kt}\cdot\Gamma(\sqrt{u})-u\log(1/u)\\
&=\frac{t}{1+2Kt}\cdot\Gamma(\sqrt{u})+u\log(u).
\end{aligned}
$$

We wish to show that $H(x,t)\leq 0$ for all $(x,t)\in V(G)\times(0,T]$. Let (x^*,t^*) be a vertex where H is maximized on $V(G)\times(0,T]$, if such a point exists. We may assume that $u(x^*,t^*)$ is not locally constant in the neighborhood of x^*, as otherwise $H(x^*,t^*)\leq 0$ and we will be done. At the maximum point, we compute

$$
\begin{aligned}
0&\geq\mathcal{L}(H)\\
&=-\frac{1}{(1+2Kt)^2}\Gamma(\sqrt{u})+\frac{2t}{1+2Kt}\tilde{\Gamma}_2(\sqrt{u})+\mathcal{L}(u\log u)\\
&\geq-\left(\frac{1}{(1+2Kt)^2}+\frac{2tK}{1+2Kt}\right)\Gamma(\sqrt{u})+\mathcal{L}(u\log u)\\
&\geq-\Gamma(\sqrt{u})+\mathcal{L}(u\log u)\\
&>0.
\end{aligned}
$$

Here, the second inequality follows from $CDE(\infty, -K)$. The third inequality follows from the fact that

$$\frac{1}{(1+2Kt)^2} + \frac{2tK}{1+2Kt} = \frac{1+(1+2Kt)2tK}{(1+2Kt)^2} \leq 1.$$

The strict inequality in the last step follows from the fact that u is not locally constant in the neighborhood of (x^*, t^*) and $CDE(\infty, -K)$ implies that $\tilde{\Gamma}_2(\sqrt{u}) \geq -K\Gamma(\sqrt{u})$. This contradiction implies that there is no maximum. On the other hand, for every vertex x

$$\lim_{t \to 0^+} H(x,t) \leq 0.$$

These combine to imply that $H(x,t) \leq 0$ everywhere.

This completes the proof. Indeed, in this case, at any point (x,t)

$$\frac{t}{1+2Kt} \cdot \Gamma(\sqrt{u}) - u\log(1/u) \leq 0,$$

so

$$\frac{\Gamma(\sqrt{u})}{u} \leq \left(\frac{1}{t} + 2K\right)\log(1/u).$$

∎

A similar statement holds for infinite graphs. In this case, however, we must be more careful in applying the maximum principle which complicates the proof somewhat.

Theorem 6. *Suppose $G = (V,E)$ is a bounded degree infinite graph satisfying $CDE(\infty, -K)$ for some $K \geq 0$, and u is a positive solution to the heat equation valid for $V(G) \times (0,\infty)$ with $||u||_\infty = 1$. Then at all $x \in V(G)$ and $t \in (0,\infty)$,*

$$\frac{\Gamma(\sqrt{u})}{u} \leq \left(\frac{1}{t} + 2K\right)\log\left(\frac{1}{u}\right),$$

Remark: Observe that we require, in this case, u to be a positive solution on the entire graph. It would also be desirable to have a version of Theorem 6 which is valid for solutions which only satisfy the heat equation on a ball of radius R (as opposed to the entire graph) as such restrictions occasionally appear in proofs. This proves to be a somewhat more tricky business, even in the continuous version. Indeed, this necessary seems to require error term involving R and $\log^2(1/u)$ as opposed to just $\log(1/u)$, and we are currently unable to prove such a version on graphs. This inequality on manifolds, due to Souplet and Zhang [18], requires a number of identities involving the chain rule beyond those which are already 'cooked in' to our method. In particular, the form of our theorem and CDE inequality is designed to overcome the fact that the identity $\Delta \log u = \frac{|\nabla u|^2}{u^2} - \frac{\Delta u}{u}$ fails for graphs. The Souplet and Zhang result in the continuous case relies on an identity for $|\nabla \log(1 - \log(u))|^2$ which fails horribly in the discrete case. On the other hand, we give a slightly stronger result than Souplet and Zhang's for solutions valid everywhere.

Proof of Theorem 6. Fix $x_0 \in V(G)$, and $T \in (0,\infty)$ and we prove that $u(x_0, T)$ satisfies the desired inequality. As calculated in the finite case, we record that at any vertex x and at any time t.

$$\mathcal{L}(u\log u)(x,t) > \Gamma(\sqrt{u})(x,t)$$

if u is not locally constant in the neighborhood of x.

Fix a positive integer $R \geq 2$, and let

$$\varphi(y) = \max\left\{1 - \frac{d(x_0, y)}{R}, 0\right\},$$

where $d(x_0, y)$ denotes the graph distance between x_0 and y.

We let

$$H = \frac{t}{1 + 2Kt} \cdot \Gamma(\sqrt{u}) + \left(1 + \frac{D_{\max} \cdot t}{\sqrt{R}}\right)(u \log u).$$

We claim that

$$H(x_0, T) \leq \frac{T \cdot D_{\max}}{\sqrt{R}}. \tag{9}$$

Assuming this holds for every positive $R \geq 2$, taking $R \to \infty$ we have that at (x_0, T)

$$\frac{T}{1 + 2KT} \cdot \Gamma(\sqrt{u}) + u \log u \leq 0,$$

and rearranging yields the result. Thus it suffices to prove (9) holds for arbitrary R. Since $\varphi(x_0) = 1$, it suffices to show that $\varphi H \leq \frac{T}{\sqrt{R}}$ for all $(x, t) \in V \times (0, T]$.

Since $\varphi H \equiv 0$ outside of $B(x_0, R)$ and $\lim_{t \to 0^+} H(x, t) \leq 0$ for every vertex $x \in V(G)$, if $\varphi H \geq \frac{T}{\sqrt{R}}$ at some (x, t), then there exists some (x^*, t^*) maximizing φH. Moreover, u cannot be constant in the neighborhood of x^* at time t^*. Note that as $||u||_\infty \leq 1$, Lemma 1 gives

$$\Gamma(\sqrt{u})(x, t) = \frac{1}{2} \widetilde{\sum_{y \sim x}} (\sqrt{u}(y) - \sqrt{u}(x))^2 \leq \frac{D_{\max}}{2}.$$

Since $u \log u \leq 0$, this means that if $\varphi H(x^*, t^*) \geq \frac{T \cdot D_{\max}}{\sqrt{R}}$, then $\varphi(x^*) \geq \frac{2}{\sqrt{R}}$.

At (x^*, t^*), then

$$\begin{aligned}
\widetilde{\sum_{y \sim x^*}} (\varphi(y) H(y, t^*) - \varphi(x^*) H(x^*, t^*)) &= \Delta(\varphi H)(x^*, t^*) \\
&\geq \mathcal{L}(\varphi H)(x^*, t^*) \\
&= \mathcal{L}(\varphi) H(x^*, t^*) + 2\Gamma(\varphi, H)(x^* t, t^*) + \varphi(x^*) \mathcal{L}(H)(x^*, t^*) \\
&= \Delta(\varphi) H(x^*, t^*) + 2\Gamma(\varphi, H)(x^*, t^*) + \varphi(x^*) \mathcal{L}(H)(x^*, t^*) \\
&= \widetilde{\sum_{y \sim x^*}} (\varphi(y) - \varphi(x^*)) H(x^*, t^*) \\
&\quad + \widetilde{\sum_{y \sim x^*}} (\varphi(y) - \varphi(x^*))(H(y, t^*) - H(x, t^*)) + \varphi(x^*) \mathcal{L}(H)(x^*, t^*) \\
&= \widetilde{\sum_{y \sim x^*}} (\varphi(y) - \varphi(x^*)) H(y, t^*) + \varphi(x^*) \mathcal{L}(H)(x^*, t^*).
\end{aligned}$$

Rearranging, we obtain

$$0 \geq \varphi(x^*) \widetilde{\sum_{y \sim x^*}} (H(x^*, t^*) - H(y, t^*)) + \varphi(x^*) \mathcal{L}(H)(x^*, t^*). \tag{10}$$

We further use that

$$\varphi(x^*)H(x^*,t^*) \geq \varphi(y)H(y,t^*),$$

and combine it with (10) to obtain

$$\begin{aligned}
0 &\geq \varphi(x^*)H(x^*,t^*)\widetilde{\sum_{y\sim x^*}}\left(1-\frac{\varphi(x^*)}{\varphi(y)}\right)+\varphi\mathcal{L}(H)(x^*,t^*)\\
&= H(x^*,t^*)\widetilde{\sum_{y\sim x^*}}(\varphi(y)-\varphi(x^*))\cdot\frac{\varphi(x^*)}{\varphi(y)}+\varphi\mathcal{L}(H)(x^*,t^*)\\
&\geq -\frac{D_{\max}}{R}H(x^*,t^*)+\varphi\mathcal{L}(H)(x^*,t^*). \qquad (11)
\end{aligned}$$

In the last line, we used Lemma 1 and the fact that

$$(\varphi(y))-\varphi(x^*))\frac{\varphi(x^*)}{\varphi(y)} = \frac{d(x_0,y)-d(x_0,x^*)}{R}\cdot\frac{R-d(x^*,x_0)}{R-d(y,x_0)} \geq -\frac{1}{R}.$$

This, in turn, follows from the fact that if $d(x_0,y)=d(x_0,x^*)-1$ (making the above negative)

$$\frac{R-d(x^*,x_0)}{R-d(y,x_0)} = \frac{R-d(x^*,x_0)}{R-d(x^*,x_0)+1} \leq 1.$$

Now we handle the $\mathcal{L}(H)$ term. Continuing from (11), we have

$$\begin{aligned}
0 &\geq \frac{-D_{\max}}{R}H(x^*,t^*)+\varphi\mathcal{L}(H)(x^*,t^*)\\
&= \frac{-D_{\max}}{R}H(x^*,t^*)+\varphi(x^*)\cdot\mathcal{L}\left(\frac{t}{1+2t^*K}\Gamma(\sqrt{u})(x^*,t^*)+u(x^*,t^*)\log u(x^*,t^*)\right)\\
&\qquad +\varphi(x^*)\mathcal{L}\left(\frac{t^*D_{\max}}{\sqrt{R}}u(x^*,t^*)\log u(x^*,t^*)\right)\\
&> \frac{-D_{\max}}{R}H(x^*,t^*)+\varphi(x^*)\left[\frac{t^*\cdot D_{\max}}{\sqrt{R}}\mathcal{L}\left(u\log u(x^*,t^*)\right)-\frac{D_{\max}}{\sqrt{R}}u\log u(x^*,t^*)\right]\\
&> \frac{-D_{\max}}{R}H(x^*,t^*)+\frac{D_{\max}\varphi(x^*)}{\sqrt{R}}\left[t\cdot\Gamma(\sqrt{u})(x^*,t^*)\right]\\
&\geq \left(\frac{\cdot D_{\max}\cdot\varphi(x^*)}{\sqrt{R}}-\frac{D_{\max}}{R}\right)H(x^*,t^*)\\
&\geq 0.
\end{aligned}$$

This contradiction implies that a maximum (x^*,t^*) of φH with $\varphi H(x^*,t^*) \geq \frac{T\cdot D_{\max}}{\sqrt{R}}$ cannot occur, and completes the proof of the theorem. In this string of inequalities, the first follows from the fact that

$$\mathcal{L}\left(t\cdot\Gamma(\sqrt{u})+u\log u\right) > 0$$

at all points where u is locally non-constant, which is the content of the proof of Theorem 5. The second inequality follows from our recorded inequality (8) above; that is that

$$\mathcal{L}\left(u\log u\right) \geq \Gamma(\sqrt{u}).$$

The third follows from the definition of H, and the final inequality follows from the fact that $\varphi(x^*) \geq \frac{2}{\sqrt{R}}$. ∎

While we have chosen to state these theorems by normalizing so that $||u||_\infty = 1$, note that by normalizing one has the immediate corollary:

COROLLARY 7. *Suppose $G = (V, E)$ is a finite or bounded degree infinite graph satisfying $CDE(\infty, -K)$ for some $K \geq 0$, and u is a positive solution to the heat equation valid for $V(G) \times (0, \infty)$ with $||u||_\infty$. Then at all $x \in V(G)$ and $t \in (0, \infty)$,*

$$\frac{\Gamma(\sqrt{u})}{u} \leq \left(\frac{1}{t} + 2K\right) \log\left(\frac{||u||_\infty}{u}\right),$$

Note also that if $||u(\cdot, t)||_\infty$ denotes the maximum heat at time t, $\frac{\partial}{\partial t}||u(\cdot, t)|| \leq 0$ so that $||u||_\infty = ||u(\cdot, 0)||_\infty$.

3. A Comparison Inequality. We now show how to use Theorems 5 and 6 in order to derive a type of multiplicative 'Harnack inequality,' comparing the heat of two different vertices at the same time. As a comparison, it is helpful tbo recall the Harnack inequality derived in [2] which is very much of the classical form. For convenience, we state it only in the simplest form (that is when the graph is unweighted, and the the vertices have measure $\mu(v) = \deg(v)$ for the definition of the Laplacian.) For a finite or infinite graph satisfying $CDE(n, 0)$, the Harnack inequality then states that

$$u(x, T_1) \leq u(y, T_2) \left(\frac{T_2}{T_1}\right)^n \exp\left(\frac{4Dd(x, y)^2}{T_2 - T_1}\right),$$

where D denotes the maximum degree of a vertex in G.

Note that the right hand side of the inequality is undefined if $T_2 = T_1$. The gradient estimate developed in this paper allows us to sidestep this issue, and derive a bound somewhat reminiscent of the above.

As a first step, we make a record a observation, in the vein of creflem:triv, which follows immediately from the definition of $\Gamma(f)$.

LEMMA 8. *Suppose $x \sim y$, and $f : V \to \mathbb{R}$*

$$(f(x) - f(y))^2 \leq \frac{\mu_{\max}}{w_{\min}} \cdot \Gamma(f)(x).$$

THEOREM 9. *Suppose $G = (V, E)$ is a (finite or bounded degree infinite) graph satisfying $CDE(\infty, -K)$ for some $K \geq 0$, and u is a positive solution to the heat equation with $||u||_\infty = 1$. Then for all $x, y \in V(G)$ and $t \in (0, \infty)$,*

$$u(x, t) \leq u(y, t) \cdot \exp\left(2d(x, y)\sqrt{\left(\frac{1}{t} + 2K\right) \cdot \frac{\mu_{\max}}{w_{\min}} \cdot \log(1/u(y, t))}\right).$$

Proof. We prove this by induction on $d(x, y)$, and further note that we may assume that

$$u(y, t) \cdot \exp\left(2d(x, y)\sqrt{\left(\frac{1}{t} + 2K\right) \cdot \frac{\mu_{\max}}{w_{\min}} \cdot \log(1/u(y, t))}\right) \leq 1,$$

as otherwise the inequality is trivial.

First, assume $x \sim y$. Then

$$\begin{aligned}
\frac{1}{2}\log\left(\frac{u(x,t)}{u(y,t)}\right) &= \log\left(\frac{\sqrt{u(x,t)}}{\sqrt{u(y,t)}}\right) \\
&\leq \frac{\sqrt{u(x,t)}-\sqrt{u(y,t)}}{\sqrt{u(y,t)}} \\
&\leq \sqrt{\frac{(\sqrt{u(x,t)}-\sqrt{u(y,t)})^2}{u(y,t)}} \\
&\leq \sqrt{\frac{\mu_{\max}}{w_{\min}}\cdot\frac{\Gamma(\sqrt{u})(y,t)}{u(y,t)}} \\
&\leq \sqrt{\left(\frac{1}{t}+2K\right)\cdot\frac{\mu_{\max}}{w_{\min}}\cdot\log\left(\frac{1}{u(y,t)}\right)}.
\end{aligned}$$

Here, the first inequality follows from the real number inequality $\log(r) \leq r-1$, the third from Lemma 8, and the last from Theorem 5 (or Theorem 6). Rearranging and exponentiating then gives the desired result in the case $d(x,y)=1$.

Now consider the general case: Suppose $d(x,y)=n\geq 2$, and consider a shortest path connecting them, $x=x_1,x_2,\dots,x_n=y$. By induction,

$$u(x_2,t) \leq u(y,t)\cdot\exp\left(2(n-1)\sqrt{\left(\frac{1}{t}+2K\right)\cdot\frac{\mu_{\max}}{w_{\min}}\cdot\log\left(\frac{1}{u(y,t)}\right)}\right).$$

Furthermore

$$u(x_1,t) \leq u(x_2,t)\cdot\exp\left(2\sqrt{\left(\frac{1}{t}+2K\right)\cdot\frac{\mu_{\max}}{w_{\min}}\cdot\log\left(\frac{1}{u(x_2,t)}\right)}\right).$$

Now consider the function

$$f(z) = z\cdot\exp(C\sqrt{\log(1/z)})$$

for some positive constant C and considered for $0\leq z\leq 1$. If f were an increasing function of z, then we could simply combine the inequalities, obtaining

$$\begin{aligned}
u(x_1,t) &\le u(x_2,t)\cdot\exp\left(2\sqrt{\left(\frac{1}{t}+2K\right)\cdot\frac{\mu_{\max}}{w_{\min}}\cdot\log\left(\frac{1}{u(x_2,t)}\right)}\right)\\
&\le u(y,t)\cdot\exp\left(2(n-1)\sqrt{\left(\frac{1}{t}+2K\right)\cdot\frac{\mu_{\max}}{w_{\min}}\cdot\log\left(\frac{1}{u(y,t)}\right)}\right)\\
&\quad\times\exp\left(2\sqrt{\left(\frac{1}{t}+2K\right)\cdot\frac{\mu_{\max}}{w_{\min}}\cdot\log\left(\frac{1}{u(y,t)\exp(\cdots)}\right)}\right)\\
&\le u(y,t)\cdot\exp\left(2(n-1)\sqrt{\left(\frac{1}{t}+2K\right)\cdot\frac{\mu_{\max}}{w_{\min}}\cdot\log\left(\frac{1}{u(y,t)}\right)}\right)\\
&\quad\times\exp\left(2\sqrt{\left(\frac{1}{t}+2K\right)\cdot\frac{\mu_{\max}}{w_{\min}}\cdot\log\left(\frac{1}{u(y,t)}\right)}\right)\\
&= u(y,t)\cdot\exp\left(2n\sqrt{\left(\frac{1}{t}+2K\right)\cdot\frac{\mu_{\max}}{w_{\min}}\cdot\log\left(\frac{1}{u(y,t)}\right)}\right). \qquad (12)
\end{aligned}$$

Here in the second inequality we use the fact that the exponential term appearing in the logarithm is at least one (as the exponent is positive). As log is increasing, discarding exponential term increases the argument in the log and hence we get the claimed inequality.

This is exactly what we claimed; and we have verified it modulo showing that f is increasing. Unfortunately, f is not a strictly increasing function, but it is unimodal which will suffice for our purposes. Note

$$f'(z)=\exp(C\sqrt{\log(1/z)})\left(1-\frac{C}{2\sqrt{\log(1/z)}}\right).$$

Thus $f(z)$ is increasing for $z\le\exp(-4/C^2)$ and then decreasing. Furthermore $f(1)=1$, and hence the maximum value of f is larger than one. To justify the last computation, we need to take $C=2(n-1)\sqrt{\left(\frac{1}{t}+2K\right)\cdot\frac{\mu_{\max}}{w_{\min}}}$ and show that

$$f(u(x_2,t))\le f\left(u(y,t)\cdot\exp\left(2(n-1)\sqrt{\left(\frac{1}{t}+2K\right)\cdot\frac{\mu_{\max}}{w_{\min}}\cdot\log\left(\frac{1}{u(y,t)}\right)}\right)\right).$$

If this *fails*, then the maximum of $f(z)$ must occur for some

$$z^*\le u(y,t)\cdot\exp\left(2(n-1)\sqrt{\left(\frac{1}{t}+2K\right)\cdot\frac{\mu_{\max}}{w_{\min}}\cdot\log\left(\frac{1}{u(y,t)}\right)}\right).$$

Since $f(z)\ge 1$ for $z^*\le z\le 1$, this means

$$f\left(u(y,t)\cdot\exp\left(2(n-1)\sqrt{\left(\frac{1}{t}+2K\right)\cdot\frac{\mu_{\max}}{w_{\min}}\cdot\log\left(\frac{1}{u(y,t)}\right)}\right)\right)>1.$$

But our computation showed that

$$f\left(u(y,t)\cdot\exp\left(2(n-1)\sqrt{\left(\frac{1}{t}+2K\right)\cdot\frac{\mu_{\max}}{w_{\min}}\cdot\log\left(\frac{1}{u(y,t)}\right)}\right)\right)$$
$$\leq u(y,t)\cdot\exp\left(2n\sqrt{\left(\frac{1}{t}+2K\right)\cdot\frac{\mu_{\max}}{w_{\min}}\cdot\log\left(\frac{1}{u(y,t)}\right)}\right),$$

which we have assumed is at most one by our hypothesis. This contradiction fully justifies (12) and proves the theorem. ∎

Normalizing u, one obtains

Corollary 10. *Suppose $G=(V,E)$ is a (finite or bounded degree infinite) graph satisfying $CDE(\infty,-K)$ for some $K\geq 0$, and u is a positive solution to the heat equation. Then for all $x,y\in V(G)$ and $t\in(0,\infty)$,*

$$u(x,t)\leq u(y,t)\cdot\exp\left(2d(x,y)\sqrt{\left(\frac{1}{t}+2K\right)\cdot\frac{\mu_{\max}}{w_{\min}}\cdot\log(||u||_\infty/u(y,t))}\right).$$

As an application, we observe that the maximum heat of a vertex in a finite graph at time t can be bounded in terms of the average heat (which is unchanging). This is most interesting when one has a non-negatively curved graph for which one obtains:

Corollary 11. *Suppose $G=(V,E)$ is an n vertex graph of diameter $\mathrm{diam}(G)$ which satisfies $CDE(\infty,0)$. Suppose $u(x,t)$ is a positive solution to the heat equation on G with $||u||_\infty=1$. Then for all $x\in V(G)$ and $t\in(0,\infty)$,*

$$u(x,t)\leq\frac{||u(\cdot,t)||_1}{n}\exp\left(2\cdot\mathrm{diam}(G)\cdot\sqrt{\frac{1}{t}\cdot\frac{\mu_{\max}}{w_{\min}}\cdot\log\left(\frac{n}{||u(\cdot,t)||_1}\right)}\right).$$

This follows immediately from taking the y in Theorem 9 to have the minimum value which is at most $||u(\cdot,t)||_1/n$ (and noting, as in the proof of Theorem 9 that if this minimum were too large to apply monotonicity, the bound above is larger than one.) Also note that this corollary holds verbatim if $||u||_\infty\leq 1$ as opposed to $||u||_\infty=1$.

We close with a final corollary related to mixing of random walks. Suppose G is an unweighted d-regular graph. As is well known, a positive solution to the heat equation with $||u(\cdot,t)||_1=1$ corresponds to the evolution of the distribution of the continuous time random walk on a graph where Δ is chosen with the measure $\mu(v)=\deg(v)$. Note that in the irregular case, it is possible to translate between the two but they are not quite identical so, for simplicity, we stick to the regular case.

For a regular graph, the stationary distribution is the uniform distribution and Corollary 11 gives a bound on how much the distribution can exceed the stationary distribution at time t. That is,

Corollary 12. *Suppose $G=(V,E)$ is a D-regular graph on n vertices, satisfying $CDE(\infty,0)$. Let $u(\cdot,t)$ denote the distribution of a continuous time random walk at time t. Then for all $x\in V(G)$ and $t\in(0,\infty)$,*

$$u(x,t)\leq\frac{1}{n}\exp\left(2\cdot\mathrm{diam}(G)\sqrt{\frac{1}{t}\cdot D\cdot\log(n)}\right).$$

Thus for non-negatively curved graphs one immediately gets a bound on the mixing rate in terms of the order of the graph, the degree and the diameter. For graphs satisfying $CDE'(n, K)$ for some $K > 0$ – which also necessarily satisfy $CDE(\infty, 0)$ – the diameter can also be bounded in terms of K (see eg. [10]) and hence one obtains a mixing rate on such graphs. Note that the corollary uses the fact that for a distribution function u, $||u||_\infty \leq 1$. Indeed if a better a priori bound on $||u||_\infty$ is available, this can be used in its stead.

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