A NOTE ON NORMALIZED HEAT DIFFUSION FOR GRAPHS

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Abstract. We show that, on graphs which have precisely three distinct Laplacian eigenvalues, heat diffusion enjoys a monotonic behaviour.

1. Introduction

Let X be a finite connected graph. The *heat kernel* on X is given by

$$H_t = e^{-tL}$$

where L is the *Laplacian* on X, and $t \geq 0$ is the time variable. In [5], Regev and Shinkar considered the question whether X has *monotonic normalized heat diffusion*: is the ratio

$$\frac{H_t(u,v)}{H_t(u,u)}$$

monotonically non-decreasing, as a function of time, for every pair of vertices u and v? Specifically, Peres (2013) had asked whether this is always the case in a vertex-transitive graph. This turns out to be too optimistic: the main result of Regev and Shinkar is that there are Cayley graphs which do not have monotonic normalized heat diffusion. On the other hand, McMurray Price [3] has shown that Cayley graphs of abelian groups do have monotonic normalized heat diffusion. In [5], Regev and Shinkar also give an example, based on an idea of Cheeger, of a regular graph which does not have monotonic normalized heat diffusion. The example is a 4-regular graph on 10 vertices, obtained as follows: consider the usual cube graph on 8 nodes, and cone off two opposite faces by two additional vertices.

The vertex-transitivity assumption in the question raised by Peres is presumably meant to enforce a constant diagonal for the heat kernel, i.e., $H_t(u,u)$ is independent of the choice of vertex u. Actually, this heat homogeneity holds if and only if X is walk-regular, see Theorem 5 in the Appendix. Notable classes of walk-regular graphs include vertex-transitive graphs; distance-regular graphs; regular graphs having at most four distinct eigenvalues. We are thus led to the question whether the latter class enjoys monotonic normalized heat diffusion.

We show the following:

Theorem 1. *If X has three distinct Laplacian eigenvalues, then X has monotonic normalized heat diffusion.*

The regular graphs with three distinct Laplacian eigenvalues are precisely the strongly regular graphs. Therefore strongly regular graphs enjoy monotonic normalized heat diffusion.

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Somewhat surprisingly, monotonic normalized heat diffusion also holds for non-regular graphs with three distinct Laplacian eigenvalues. Our favourite example of such a graph is the so-called *Erdős - Rényi orthogonality graph*. Given a finite field $\mathbb{F}$ with q elements, the graph ER_q has the projective plane $PG(2,\mathbb{F}) = (\mathbb{F}^3)^*/\mathbb{F}$ as its vertex set as its vertex set. Two distinct vertices $[x_1, x_2, x_3]$ and $[y_1, y_2, y_3]$ are joined by an edge whenever $x_1y_1 + x_2y_2 + x_3y_3 = 0$. The graph ER_q has q^2+q+1 vertices; q^2 of them have degree $q+1$, and the remaining $q+1$ have degree q. The Laplacian eigenvalues of ER_q are 0, and $q+1\pm\sqrt{q}$. Historically, the Erdős - Rényi graph first appeared in Turán-type extremal graph theory, as a graph with many edges but no 4-cycles. We refer to [4, Ch.12] for details. Several other constructions of non-regular graphs with three distinct Laplacian eigenvalues are studied in [1].

We conclude this preamble by raising the following problem: do regular graphs with four distinct eigenvalues enjoy monotonic normalized heat diffusion? It is likely that this problem can be handled by a strategy similar to the one employed below, but the computations are quite unwieldy.

2. Preliminaries

Let X be a finite connected graph, having at least two vertices. The Laplacian on X is a symmetric linear operator on the space of real-valued functions defined on the vertex set V of X. This is a finite-dimensional space, endowed with the inner product

$$\langle \phi, \psi \rangle = \sum_{v\in V} \phi(v)\, \psi(v).$$

The Laplacian, denoted by L, has matrix coefficients $L(u,v) = \langle L\mathbb{1}_v, \mathbb{1}_u\rangle$, where $u, v \in V$, given as follows: off-diagonally, $L(u,v) = 0$ if $u \neq v$ are not adjacent, respectively $L(u,v) = -1$ if $u \neq v$ are adjacent; diagonally, $L(u,u) = \deg(u)$, the degree of u.

Let $n = |V|$ denote the number of vertices of X. Then L has n non-negative eigenvalues, counted with multiplicities. The trivial eigenvalue $\lambda = 0$ admits the constant function $\mathbb{1}$ as an eigenfunction, and it is simple thanks to connectivity. On the other hand, the non-trivial eigenvalues can, and usually do, have a high multiplicity.

Let $\sigma(L)$ denote the set of distinct eigenvalues of L. We then have the spectral decomposition

$$L = \sum_{\lambda\in\sigma(L)} \lambda\, P_\lambda$$

where P_λ denotes the projection onto the λ-eigenspace. The projection P_0, corresponding to the trivial eigenvalue, is the averaging operator $P_0\phi = \frac{1}{n}\sum_{v\in V}\phi(v)$. In terms of matrix coefficients, we have $P_0(u,v) = \frac{1}{n}$ for all $u, v \in V$.

The spectral decomposition for the Laplacian induces, by functional calculus, a spectral decomposition for the heat kernel:

$$H_t = e^{-tL} = \sum_{\lambda\in\sigma(L)} e^{-t\lambda}\, P_\lambda$$

for all $t \geq 0$. This formula makes it apparent that the heat kernel evolves from $I = H_0$ towards $P_0 = \lim_{t\to\infty} H_t$. We will make significant use of the spectral decomposition of the heat kernel, a perspective that is quite different from the approaches taken in [5, 3].

3. Proof of Theorem 1

We start with two facts that hold without any spectral hypothesis on X. The first one is a well-known bound relating vertex degrees and Laplacian eigenvalues.

Lemma 2. *The degree of each vertex u satisfies*

$$\min_{0\neq\lambda\in\sigma(L)} \lambda \leq \deg(u), \qquad \deg(u)+1 \leq \max_{\lambda\in\sigma(L)} \lambda.$$

The second fact says that normalized heat diffusion starts off in a non-decreasing way.

Lemma 3. *For any pair of distinct vertices u and v, the normalized heat diffusion*

$$\frac{H_t(u,v)}{H_t(u,u)}$$

has non-negative derivative at $t=0$.

Proof. We need to show that

$$H_t'(u,v)H_t(u,u) \geq H_t(u,v)H_t'(u,u)$$

at $t=0$. We have $H_0(u,u)=1$ and $H_0(u,v)=0$, since $H_0=I$, so we are left with checking that $H_0'(u,v)\geq 0$. Now, $H_t'=-LH_t$, in particular $H_0'=-LH_0=-L$. Hence $H_0'(u,v)=-L(u,v)\geq 0$, as desired. □

Assume now that X has three distinct Laplacian eigenvalues, say $0<\theta_1<\theta_2$. Then the heat kernel is given by

$$H_t = P_0 + e^{-t\theta_1}\, P_{\theta_1} + e^{-t\theta_2}\, P_{\theta_2}.$$

Let u and v be distinct vertices of X. In order to prove Theorem 1, we have to check that the function

$$h(t) := H_t'(u,v)H_t(u,u) - H_t(u,v)H_t'(u,u)$$

satisfies $h(t)\geq 0$ at all times $t\geq 0$. One computes

(∗)

$$e^{t(\theta_1+\theta_2)}\, h(t) = \frac{\theta_1}{n}\big(P_{\theta_1}(u,u)-P_{\theta_1}(u,v)\big)\, e^{t\theta_2} + \frac{\theta_2}{n}\big(P_{\theta_2}(u,u)-P_{\theta_2}(u,v)\big)\, e^{t\theta_1} - R$$

where the remainder R is explicitly given as

$$R = (\theta_1-\theta_2)\big(P_{\theta_1}(u,u)\, P_{\theta_2}(u,v) - P_{\theta_1}(u,v)\, P_{\theta_2}(u,u)\big).$$

Importantly, note that the remainder R is independent of t.

Lemma 4. *$P_{\theta_1}(u,u)\geq P_{\theta_1}(u,v)$ and $P_{\theta_2}(u,u)\geq P_{\theta_2}(u,v)$.*

This lemma addresses the coefficients appearing on the right-hand side of (∗). It follows that $g(t)=e^{t(\theta_1+\theta_2)}\, h(t)$ is increasing, and so $g(t)\geq g(0)=h(0)$ for all $t\geq 0$. As $h(0)\geq 0$, by Lemma 3, we deduce that $h(t)\geq 0$ for all $t\geq 0$.

Proof of Lemma 4. The two projections, P_{θ_1} and P_{θ_2}, can be determined from the following system:

$$P_{\theta_1} + P_{\theta_2} = I - P_0$$
$$\theta_1 P_{\theta_1} + \theta_2 P_{\theta_2} = L.$$

The solution is

$$P_{\theta_1} = \frac{L - \theta_2(I - P_0)}{\theta_1 - \theta_2}, \qquad P_{\theta_2} = \frac{L - \theta_1(I - P_0)}{\theta_2 - \theta_1}.$$

Then one computes

$$P_{\theta_1}(u,u) - P_{\theta_1}(u,v) = \frac{\deg(u) - \theta_2 - L(u,v)}{\theta_1 - \theta_2},$$
$$P_{\theta_2}(u,u) - P_{\theta_2}(u,v) = \frac{\deg(u) - \theta_1 - L(u,v)}{\theta_2 - \theta_1}.$$

Lemma 2 says, for the case at hand, that $\theta_1 \leq \deg(u)$, and $\deg(u) + 1 \leq \theta_2$. It follows that $\deg(u) - \theta_1 - L(u,v) \geq 0$, and $\deg(u) - \theta_2 - L(u,v) \leq 0$. This proves the claim of the lemma. □

4. Appendix: Walk-regular graphs

A graph is *walk regular* if, for each $k \geq 2$, the number of closed walks of length ℓ starting and ending at a vertex is independent of the choice of vertex. Taking $\ell = 2$, we see that a walk-regular graph is, in particular, regular. The notion of walk regularity, as well as some of its basic properties, first appeared in [2].

Theorem 5. *The following are equivalent:*

- (X) *X is walk-regular;*
- (A) *A^k has constant diagonal, for all $k = 0, 1, \ldots$;*
- (L) *L^k has constant diagonal, for all $k = 0, 1, \ldots$;*
- (H) *H_t has constant diagonal, for all $t \geq 0$;*
- (P) *P_λ has constant diagonal, for all $\lambda \neq 0$.*

Proof. The equivalence of (X) and (A), already noted in [2], owes to the fact that $A^k(u,u)$ counts the number of closed walks of length k starting and ending at a vertex u.

The equivalence of (A) and (L) owes, firstly, to the regularity of X, expressed by the value $k = 2$ in (A), respectively the value $k = 1$, or $k = 2$, in (L). Then the relation $A + L = dI$, where d is the degree of X, leads to A^k being a polynomial of degree k in L, respectively L^k being a polynomial of degree k in A.

The equivalence of (L) and (H) is based on the power series formula

$$H_t(u,u) = \sum_{k=0}^{\infty} \frac{(-1)^k L^k(u,u)}{k!}\, t^k$$

for each vertex u, and all times $t \geq 0$. If (L) holds, then the right-hand side is independent of u, and (H) follows. If (H) holds, then the left-hand side is independent of u, so it can be seen as a function of t only. By the uniqueness of a power series expansion, $L^k(u,u)$ is independent of u, for all $k = 0, 1, \ldots$.

The equivalence of (H) and (P) is based on the formula

$$H_t(u,u) = \sum_{\lambda \in \sigma(L)} e^{-t\lambda}\, P_\lambda(u,u)$$

for each vertex u, and all times $t \geq 0$. Clearly, then, (P) implies (H). The converse implication owes to the fact that the scaled exponentials $t \mapsto e^{-t\lambda}$, for λ running over $\sigma(L)$, are linearly independent. $\square$

From a heat kernel perspective, the main upshot is the equivalence of (X) and (H): a graph is walk-regular if and only if its heat kernel has constant diagonal at all times.

The verification of walk-regularity, on the other hand, often exploits the equivalence of (X) and (A). For example, walk-regularity for distance-regular graphs can be shown in this way [2]. Let us illustrate this perspective by discussing walk-regularity for regular graphs with few eigenvalues. If X is a regular graph with s distinct eigenvalues, then there is a monic polynomial p of degree $s-1$, the so-called Hoffman polynomial of X, with the property that the matrix $p(A)$ has constant entries. It follows that the walk-regularity of X is equivalent to A^s having constant diagonal for all $k = 0, \dots, s-2$. When $s = 3$ or $s = 4$, this clearly holds.

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