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A NOTE ON NORMALISED 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.

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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 of whether X has *monotonic normalised heat diffusion*: that is, whether the ratio

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

is monotonically nondecreasing, as a function of time, for every pair of vertices u and v. 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 normalised heat diffusion. On the other hand, McMurray Price [3] has shown that Cayley graphs of abelian groups do have monotonic normalised 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 normalised heat diffusion. The example is a 4-regular graph on 10 vertices, obtained as follows: consider the usual cube graph on eight 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, that is, $H_t(u, u)$ is independent of the choice of vertex u. This heat homogeneity holds if and only if X is walk regular (see Theorem A.1 in the Appendix). Notable classes of walk-regular graphs include vertex-transitive graphs, distance-regular graphs and regular graphs having at most four distinct eigenvalues. We are thus led to the question of whether the latter class enjoys monotonic normalised heat diffusion.

We obtain the following result.

THEOREM 1.1. *If X has three distinct Laplacian eigenvalues, then X has monotonic normalised heat diffusion.*

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

Somewhat surprisingly, monotonic normalised heat diffusion also holds for nonregular 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. 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 (see [4, Ch. 12] for details). Several other constructions of nonregular graphs with three distinct Laplacian eigenvalues were studied in [1].

We conclude this preamble by posing the following problem: do regular graphs with four distinct eigenvalues enjoy monotonic normalised 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 $L(u, v) = \langle L\mathbb{1}_v, \mathbb{1}_u \rangle$, for $u, v \in V$, given as follows: off-diagonally, $L(u, v) = 0$ if $u \neq v$ are not adjacent and $L(u, v) = -1$ 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 nonnegative 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 nontrivial eigenvalues can, and usually do, have a high multiplicity.

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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 just the averaging operator given by $P_0\phi = (1/n)\sum_{v\in V}\phi(v)$. In terms of matrix coefficients, $P_0(u, v) = 1/n$ 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 $t \geq 0$. This formula makes it apparent that the heat kernel evolves from $I = H_0$ towards $P_0 = \lim_{t\to\infty} H_t$. We make significant use of the spectral decomposition of the heat kernel, a perspective that is quite different from the approaches taken in [3, 5].

3. Proof of Theorem 1.1

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 3.1. *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 normalised heat diffusion starts off in a nondecreasing way.

Lemma 3.2. *For any pair of distinct vertices u and v, the normalised heat diffusion*

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

has nonnegative 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, $H'_t = -LH_t$ and, 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

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

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Let u and v be distinct vertices of X. In order to prove Theorem 1.1, 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

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

where the remainder R is explicitly given by

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

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

Lemma 3.3. *$P_{\theta_1}(u,u) \geq P_{\theta_1}(u,v)$ 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 3.2, we deduce that $h(t) \geq 0$ for all $t \geq 0$.

Proof of Lemma 3.3. 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

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

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 3.1 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 lemma.

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].

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THEOREM A.1. *The following are equivalent:*

(X) *X is walk regular;*
(A) *A^k has constant diagonal for all $k = 0, 1, \dots$;*
(L) *L^k has constant diagonal for all $k = 0, 1, \dots$;*
(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], comes from 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) is due, 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 $k = 0, 1, \dots$.

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 comes from the fact that the scaled exponentials $t \mapsto e^{-t\lambda}$, for λ running over $\sigma(L)$, are linearly independent. □

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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