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A NOTE ON A DISTANCE BOUND USING EIGENVALUES OF THE NORMALIZED LAPLACIAN MATRIX*

STEVE KIRKLAND[†]

Abstract. Let G be a connected graph, and let X and Y be subsets of its vertex set. A previously published bound is considered that relates the distance between X and Y to the eigenvalues of the normalized Laplacian matrix for G , the volumes of X and Y , and the volumes of their complements. A counterexample is given to the bound, and then a corrected version of the bound is provided.

Key words. Normalized Laplacian matrix, Eigenvalue, Distance.

AMS subject classifications. 05C50, 15A18.

1. Introduction. Suppose that G is a connected graph on n vertices; let A be its adjacency matrix, and let D denote the diagonal matrix of vertex degrees. The *normalized Laplacian matrix* for G , denoted \mathcal{L} , is given by $\mathcal{L} = I - D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$. It turns out that \mathcal{L} is a positive semidefinite matrix, having 0 as a simple eigenvalue (see [1]). Denote the eigenvalues of \mathcal{L} by $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_{n-1}$. The relationship between the structural properties of G and the eigenvalues of \mathcal{L} has received much attention, and the monograph [1] provides a comprehensive survey of results on that subject.

Given two nonempty subsets X, Y of the vertex set of G , the *distance* between X and Y is defined as $d(X, Y) = \min\{d(x, y) | x \in X, y \in Y\}$, where for vertices x and y , $d(x, y)$ is the length of a shortest path between x and y . The *volume* of X , denoted $vol(X)$, is defined as the sum of the degrees of the vertices in X , while $vol(G)$ denotes the sum of the degrees of all of the vertices in G . We use \bar{X} to denote the set of vertices not in X .

The following inequality relating $d(X, Y)$ to the eigenvalues of \mathcal{L} , appears in [1].

ASSERTION 1.1. ([1], Theorem 3.1) *Suppose that G is not a complete graph. Let X and Y be subsets of the vertex set of G with $X \neq Y, \bar{Y}$. Then we have*

$$(1.1) \quad d(X, Y) \leq \left\lceil \frac{\log \sqrt{\frac{vol(\bar{X})vol(\bar{Y})}{vol(X)vol(Y)}}}{\log \frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1}} \right\rceil.$$

Unfortunately, Assertion 1.1 is in error, as the following example shows.

EXAMPLE 1.2. Suppose that $p, q \in \mathbb{N}$, and let $H(p, q) = O_p \vee K_q$, where O_p is the graph on p vertices with no edges, and where $G_1 \vee G_2$ denotes the join of the graphs G_1 and G_2 . Evidently $H(p, q)$ has p vertices of degree q and q vertices of degree $p + q - 1$. Let J denote an all-ones matrix (whose order is to be taken from

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the context). The normalized Laplacian for $H(p, q)$ is given by

$$\left[\begin{array}{c|c} I & \frac{-1}{\sqrt{q(p+q-1)}} J \\ \hline \frac{-1}{\sqrt{q(p+q-1)}} J & \frac{p+q}{p+q-1} I - \frac{1}{p+q-1} J \end{array} \right].$$

The eigenvalues are readily seen to be $0, 1$ (with multiplicity $p - 1$), $\frac{p+q}{p+q-1}$ (with multiplicity $q - 1$) and $1 + \frac{p}{p+q-1}$. Hence, for $H(p, q)$ we have $\frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1} = 3 + \frac{2q-2}{p}$.

Suppose that p is even. Let X denote a set of $\frac{p}{2}$ vertices of degree q , and let Y denote the set of the remaining $\frac{p}{2}$ vertices of degree q . Note that $X \neq \bar{Y}$ and that $d(X, Y) = 2$. We have $\text{vol}(X) = \frac{qp}{2} = \text{vol}(Y)$ and $\text{vol}(\bar{X}) = q(\frac{3p}{2} + q - 1) = \text{vol}(\bar{Y})$. Consequently, $\sqrt{\frac{\text{vol}(\bar{X})\text{vol}(\bar{Y})}{\text{vol}(X)\text{vol}(Y)}} = \frac{q(\frac{3p}{2} + q - 1)}{\frac{qp}{2}} = 3 + \frac{2q-2}{p}$. Hence we have

$$\left\lceil \frac{\log \sqrt{\frac{\text{vol}(\bar{X})\text{vol}(\bar{Y})}{\text{vol}(X)\text{vol}(Y)}}}{\log \frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1}} \right\rceil = 1 < 2 = d(X, Y), \text{ contrary to Assertion 1.1.}$$

Our goal in this paper is to adapt the approach to Assertion 1.1 outlined in [1] so as to produce an amended upper bound on $d(X, Y)$. It will transpire that only a minor modification of (1.1) is needed. Needless to say, the line of thought pursued in [1] is fundamental to the present work.

Henceforth, we take G to be a connected graph on n vertices, and we take X, Y to be nonempty subsets of its vertex set, such that $X \neq Y, \bar{Y}$. Let $\mathcal{L} = I - D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$ be the normalized Laplacian matrix for G , where A is the adjacency matrix and D is the diagonal matrix of vertex degrees; denote the eigenvalues of \mathcal{L} by $0 = \lambda_0 < \lambda_1 \leq \dots \leq \lambda_{n-1}$, and let v_0, \dots, v_{n-1} denote an orthonormal basis of eigenvectors of \mathcal{L} , where for each j , v_j corresponds to λ_j . Let ψ_X denote the vector of order n with a 1 in the position corresponding to vertex i if $i \in X$ and a 0 there otherwise. We define ψ_Y analogously. Let $\mathbf{1}$ denote an all-ones vector of order n .

2. Amending the bound. We begin by analysing the argument in [1] advanced to support Assertion 1.1. We express $D^{\frac{1}{2}}\psi_X$ and $D^{\frac{1}{2}}\psi_Y$ as linear combinations of eigenvectors, say $D^{\frac{1}{2}}\psi_X = a_0 v_0 + \sum_{i=1}^{n-1} a_i v_i$ and $D^{\frac{1}{2}}\psi_Y = b_0 v_0 + \sum_{i=1}^{n-1} b_i v_i$. Since $v_0 = \frac{1}{\sqrt{\text{vol}(G)}} D^{\frac{1}{2}}\mathbf{1}$, it is straightforward to see that $a_0 = \frac{\text{vol}(X)}{\sqrt{\text{vol}(G)}}$ and $b_0 = \frac{\text{vol}(Y)}{\sqrt{\text{vol}(G)}}$.

Let $p_t(x) = (1 - \frac{2x}{\lambda_{n-1} + \lambda_1})^t$, and for each $t \in \mathbb{N}$, let $p_t(\mathcal{L})$ denote the matrix $(I - \frac{2}{\lambda_{n-1} + \lambda_1} \mathcal{L})^t$. The argument in [1] proceeds via the following approach: if for some $t \in \mathbb{N}$, the inner product $\langle D^{\frac{1}{2}}\psi_Y, p_t(\mathcal{L})D^{\frac{1}{2}}\psi_X \rangle$ is positive, then we can conclude that $d(X, Y) \leq t$. Note that for each $x \in [\lambda_1, \lambda_{n-1}]$, $|p_t(x)| \leq (\frac{\lambda_{n-1} - \lambda_1}{\lambda_{n-1} + \lambda_1})^t$. Observe that

$$\begin{aligned} \langle D^{\frac{1}{2}}\psi_Y, p_t(\mathcal{L})D^{\frac{1}{2}}\psi_X \rangle &= a_0 b_0 + \sum_{i=1}^{n-1} p_t(\lambda_i) a_i b_i \\ (2.1) \quad &\geq a_0 b_0 - \left(\frac{\lambda_{n-1} - \lambda_1}{\lambda_{n-1} + \lambda_1} \right)^t \sqrt{\sum_{i=1}^{n-1} a_i^2 \sum_{i=1}^{n-1} b_i^2} \end{aligned}$$

$$= \frac{\text{vol}(X)\text{vol}(Y)}{\text{vol}(G)} - \left(\frac{\lambda_{n-1}-\lambda_1}{\lambda_{n-1}+\lambda_1}\right)^t \frac{\sqrt{\text{vol}(X)\text{vol}(\overline{X})\text{vol}(Y)\text{vol}(\overline{Y})}}{\text{vol}(G)}.$$

At this point, it is stated in [1] (erroneously) that the inequality in (2.1) must be strict, since if equality were to hold, then there would be some constant c such that $b_i = ca_i$ for all $i = 1, \dots, n-1$, which would then imply that either $X = Y$ or $X = \overline{Y}$, contrary to hypothesis. (It turns that there are circumstances other than $X = Y$ or $X = \overline{Y}$ under which strict inequality in (2.1) fails to hold, as illustrated by Example 1.2.) Under the assumption that (2.1) is strict, it is then enough to take

$$t \geq \frac{\log \sqrt{\frac{\text{vol}(\overline{X})\text{vol}(\overline{Y})}{\text{vol}(X)\text{vol}(Y)}}}{\log \frac{\lambda_{n-1}+\lambda_1}{\lambda_{n-1}-\lambda_1}}$$

in order to conclude that $\langle D^{\frac{1}{2}}\psi_Y, p_t(\mathcal{L})D^{\frac{1}{2}}\psi_X \rangle$ is strictly positive.

Next, we discuss the case of equality in (2.1).

THEOREM 2.1. *Suppose that $X \neq Y, \overline{Y}$, and let $c = \sqrt{\frac{\text{vol}(Y)\text{vol}(\overline{Y})}{\text{vol}(X)\text{vol}(\overline{X})}}$. Suppose that $\sum_{i=1}^{n-1} p_t(\lambda_i)a_i b_i = -\left(\frac{\lambda_{n-1}-\lambda_1}{\lambda_{n-1}+\lambda_1}\right)^t \sqrt{\sum_{i=1}^{n-1} a_i^2 \sum_{i=1}^{n-1} b_i^2}$. Then there are constants α, β , and unit eigenvectors w and u , corresponding to λ_1 and λ_{n-1} , respectively, such that*

$$(2.2) \quad D^{\frac{1}{2}}\psi_X = a_0 v_0 + \alpha w + \beta u, \text{ and}$$

$$(2.3) \quad D^{\frac{1}{2}}\psi_Y = b_0 v_0 - c\alpha w + c\beta u.$$

Further, t is odd.

Proof: Since

$$(2.4) \quad \begin{aligned} \sum_{i=1}^{n-1} p_t(\lambda_i)a_i b_i &\geq -\left(\frac{\lambda_{n-1}-\lambda_1}{\lambda_{n-1}+\lambda_1}\right)^t \sum_{i=1}^{n-1} |a_i||b_i| \\ &\geq -\left(\frac{\lambda_{n-1}-\lambda_1}{\lambda_{n-1}+\lambda_1}\right)^t \sqrt{\sum_{i=1}^{n-1} a_i^2 \sum_{i=1}^{n-1} b_i^2}, \end{aligned}$$

our hypothesis implies that equality must hold throughout (2.4). In particular, since equality holds in the second inequality of (2.4), there is a constant $\hat{c} \geq 0$ such that for each $i = 1, \dots, n-1$ either $b_i = \hat{c}a_i$ or $b_i = -\hat{c}a_i$. Since $X \neq Y, \overline{Y}$, it cannot be the case that $b_i = \hat{c}a_i$ for all $i = 1, \dots, n-1$, nor can it be the case that $b_i = -\hat{c}a_i$ for all $i = 1, \dots, n-1$. In particular, we see that \hat{c} must be positive.

Further, since equality holds in the first inequality of (2.4), we must also have $p_t(\lambda_i)a_i b_i = -\left(\frac{\lambda_{n-1}-\lambda_1}{\lambda_{n-1}+\lambda_1}\right)^t |a_i||b_i|$ for each $i = 1, \dots, n-1$. Hence for each i such that $\lambda_i \neq \lambda_1, \lambda_{n-1}$, we have $a_i = b_i = 0$. Since $p_t(\lambda_1) = \left(\frac{\lambda_{n-1}-\lambda_1}{\lambda_{n-1}+\lambda_1}\right)^t$, we find that for each index i such that $\lambda_i = \lambda_1$, we must have $b_i = -\hat{c}a_i$. Also, since $p_t(\lambda_{n-1}) = (-1)^t \left(\frac{\lambda_{n-1}-\lambda_1}{\lambda_{n-1}+\lambda_1}\right)^t$, and since there is at least one index i such that $\lambda_i = \lambda_{n-1}$ and

$b_i = \hat{c}a_i \neq 0$, we find that t must be odd. It now follows that for every i such that $\lambda_i = \lambda_{n-1}$, we have $b_i = \hat{c}a_i$.

Consequently, there is a λ_1 -eigenvector w of norm 1 and a λ_{n-1} -eigenvector u of norm 1 and constants α, β such that $D^{\frac{1}{2}}\psi_X = a_0v_0 + \alpha w + \beta u$ and $D^{\frac{1}{2}}\psi_Y = b_0v_0 - \hat{c}\alpha w + \hat{c}\beta u$. Note that $\alpha \neq 0$ and $\beta \neq 0$, otherwise it follows that either $X = Y$ or $X = \bar{Y}$. It is straightforward to determine that $\alpha^2 + \beta^2 = \frac{\text{vol}(X)\text{vol}(\bar{X})}{\text{vol}(G)}$ and $\hat{c}^2\alpha^2 + \hat{c}^2\beta^2 = \frac{\text{vol}(Y)\text{vol}(\bar{Y})}{\text{vol}(G)}$, which yields $\hat{c} = \sqrt{\frac{\text{vol}(Y)\text{vol}(\bar{Y})}{\text{vol}(X)\text{vol}(\bar{X})}} = c$. \square

REMARK 2.2. Suppose that $X \cap Y = \emptyset$, and that (2.2) and (2.3) hold. Since $\langle D^{\frac{1}{2}}\psi_X, D^{\frac{1}{2}}\psi_Y \rangle = 0$, we have $a_0b_0 - c(\alpha^2 - \beta^2) = 0$. Substituting our expressions for a_0 and b_0 yields $\alpha^2 - \beta^2 = \frac{\text{vol}(X)\text{vol}(Y)}{\text{vol}(G)} \sqrt{\frac{\text{vol}(X)\text{vol}(\bar{X})}{\text{vol}(Y)\text{vol}(\bar{Y})}}$. As noted in the proof of Theorem 2.1, $\alpha^2 + \beta^2 = \frac{\text{vol}(X)\text{vol}(\bar{X})}{\text{vol}(G)}$, and so we find that $\alpha^2 = \frac{\text{vol}(X)\text{vol}(\bar{X})}{2\text{vol}(G)} \left(1 + \sqrt{\frac{\text{vol}(X)\text{vol}(Y)}{\text{vol}(\bar{X})\text{vol}(\bar{Y})}}\right)$ and $\beta^2 = \frac{\text{vol}(X)\text{vol}(\bar{X})}{2\text{vol}(G)} \left(1 - \sqrt{\frac{\text{vol}(X)\text{vol}(Y)}{\text{vol}(\bar{X})\text{vol}(\bar{Y})}}\right)$. In particular, $\alpha^2 > \beta^2$.

Since X and Y are disjoint, it follows that $d(X, Y)$ is the minimum $k \in \mathbb{N}$ such that $\langle D^{\frac{1}{2}}\psi_Y, \mathcal{L}^k D^{\frac{1}{2}}\psi_X \rangle \neq 0$. For each $k \in \mathbb{N}$ we have $\langle D^{\frac{1}{2}}\psi_Y, \mathcal{L}^k D^{\frac{1}{2}}\psi_X \rangle = -c\alpha^2\lambda_1^k + c\beta^2\lambda_{n-1}^k$. If $d(X, Y) \neq 1$, then we have $-c\alpha^2\lambda_1 + c\beta^2\lambda_{n-1} = 0$, so that $\lambda_1 = \frac{\beta^2}{\alpha^2}\lambda_{n-1}$. Hence $-c\alpha^2\lambda_1^2 + c\beta^2\lambda_{n-1}^2 = c\lambda_{n-1}^2 \frac{\beta^2}{\alpha^2}(\alpha^2 - \beta^2) > 0$. Thus, if $d(X, Y) \neq 1$ then necessarily $d(X, Y) = 2$, or equivalently, $d(\bar{X}, Y) \leq 2$.

We are now able to provide an upper bound on $d(X, Y)$ that serves as a corrected version of Assertion 1.1. From the bound below, we see that in fact (1.1) can only fail when $\sqrt{\frac{\text{vol}(\bar{X})\text{vol}(\bar{Y})}{\text{vol}(X)\text{vol}(Y)}} \leq \frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1}$.

THEOREM 2.3. *Suppose that G is not a complete graph. Let X and Y be subsets of the vertex set of G with $X \neq Y, \bar{Y}$. Then $d(X, Y) \leq \max\left\{\left\lceil \frac{\log \sqrt{\frac{\text{vol}(\bar{X})\text{vol}(\bar{Y})}{\text{vol}(X)\text{vol}(Y)}}}{\log \frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1}} \right\rceil, 2\right\}$.*

Proof: Let $t = \left\lceil \frac{\log \sqrt{\frac{\text{vol}(\bar{X})\text{vol}(\bar{Y})}{\text{vol}(X)\text{vol}(Y)}}}{\log \frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1}} \right\rceil$. If $t > \frac{\log \sqrt{\frac{\text{vol}(\bar{X})\text{vol}(\bar{Y})}{\text{vol}(X)\text{vol}(Y)}}}{\log \frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1}}$, then it follows from (2.1) that $\langle D^{\frac{1}{2}}\psi_Y, p_t(\mathcal{L})D^{\frac{1}{2}}\psi_X \rangle > 0$, and hence that $d(X, Y) \leq t$.

Henceforth we assume that the integer t is equal to $\frac{\log \sqrt{\frac{\text{vol}(\bar{X})\text{vol}(\bar{Y})}{\text{vol}(X)\text{vol}(Y)}}}{\log \frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1}}$. If strict inequality holds in (2.1), then again we conclude that $d(X, Y) \leq t$. On the other hand, if equality holds in (2.1), then from Theorem 2.1 and Remark 2.2, we have $d(X, Y) \leq 2$. The conclusion now follows. \square

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