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

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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.

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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 $\mathcal{L} = I - D^{\frac{-1}{2}} A D^{\frac{-1}{2}}$. 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 $0 = \lambda_0 < \lambda_1 \le \lambda_2 \le \ldots \le \lambda_{n-1}$. 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 $\overline{X}$ 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 $X \ne Y, \overline{Y}$. Then we have*

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

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 $X \neq \overline{Y}$ and that $d(X,Y) = 2$. We have $vol(X) = \frac{qp}{2} = vol(Y)$ and $vol(\overline{X}) = q(\frac{3p}{2}+q-1) = vol(\overline{Y})$. Consequently, $\sqrt{\frac{vol(\overline{X})vol(\overline{Y})}{vol(X)vol(Y)}} = \frac{q(\frac{3p}{2}+q-1)}{\frac{qp}{2}} = 3+\frac{2q-2}{p}$. Hence we have $\lceil \frac{\log\sqrt{\frac{vol(\overline{X})vol(\overline{Y})}{vol(X)vol(Y)}}}{\log\frac{\lambda_{n-1}+\lambda_1}{\lambda_{n-1}-\lambda_1}} \rceil = 1 < 2 = d(X,Y)$, 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 $X \neq Y, \overline{Y}$. Let $\mathcal{L} = I - D^{\frac{-1}{2}}AD^{\frac{-1}{2}}$ 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 $0 = \lambda_0 < \lambda_1 \leq \ldots \leq \lambda_{n-1}$, and let $v_0, \ldots, v_{n-1}$ 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 $D^{\frac{1}{2}}\psi_X = a_0v_0 + \sum_{i=1}^{n-1} a_iv_i$ and $D^{\frac{1}{2}}\psi_Y = b_0v_0 + \sum_{i=1}^{n-1} b_iv_i$. Since $v_0 = \frac{1}{\sqrt{vol(G)}}D^{\frac{1}{2}}\mathbf{1}$, it is straightforward to see that $a_0 = \frac{vol(X)}{\sqrt{vol(G)}}$ and $b_0 = \frac{vol(Y)}{\sqrt{vol(G)}}$.

Let $p_t(x) = (1-\frac{2x}{\lambda_{n-1}+\lambda_1})^t$, and for each $t \in I\!N$, 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 $t \in I\!N$, the inner product $< D^{\frac{1}{2}}\psi_Y, p_t(\mathcal{L})D^{\frac{1}{2}}\psi_X >$ is positive, then we can conclude that $d(X,Y) \leq t$. Note that for each $x \in [\lambda_1, \lambda_{n-1}], |p_t(x)| \leq \left(\frac{\lambda_{n-1}-\lambda_1}{\lambda_{n-1}+\lambda_1}\right)^t$. Observe that

$$< D^{\frac{1}{2}}\psi_Y, p_t(\mathcal{L})D^{\frac{1}{2}}\psi_X >= a_0b_0 + \sum_{i=1}^{n-1} p_t(\lambda_i)a_ib_i$$

$$\geq a_0b_0 - \left(\frac{\lambda_{n-1}-\lambda_1}{\lambda_{n-1}+\lambda_1}\right)^t \sqrt{\sum_{i=1}^{n-1} a_i^2 \sum_{i=1}^{n-1} b_i^2} \tag{2.1}$$

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

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 $i = 1, \ldots, n-1$, 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

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

in order to conclude that $< D^{\frac{1}{2}}\psi_Y, p_t(\mathcal{L})D^{\frac{1}{2}}\psi_X >$ 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 $c = \sqrt{\frac{vol(Y)vol(\overline{Y})}{vol(X)vol(\overline{X})}}$. Suppose that $\sum_{i=1}^{n-1} p_t(\lambda_i)a_ib_i = -\left(\frac{\lambda_{n-1}-\lambda_1}{\lambda_{n-1}+\lambda_1}\right)^t \sqrt{\sum_{i=1}^{n-1} a_i^2 \sum_{i=1}^{n-1} b_i^2}$. Then there are constants α, β, and unit eigenvectors w and u, corresponding to λ_1 and λ_{n-1}, respectively, such that*

$$D^{\frac{1}{2}}\psi_X = a_0v_0 + \alpha w + \beta u, \text{ and} \tag{2.2}$$

$$D^{\frac{1}{2}}\psi_Y = b_0v_0 - c\alpha w + c\beta u. \tag{2.3}$$

Further, t is odd.

Proof: Since

$$\sum_{i=1}^{n-1} p_t(\lambda_i)a_ib_i \geq -\left(\frac{\lambda_{n-1}-\lambda_1}{\lambda_{n-1}+\lambda_1}\right)^t \sum_{i=1}^{n-1} |a_i||b_i|$$

$$\geq -\left(\frac{\lambda_{n-1}-\lambda_1}{\lambda_{n-1}+\lambda_1}\right)^t \sqrt{\sum_{i=1}^{n-1} a_i^2 \sum_{i=1}^{n-1} b_i^2}, \tag{2.4}$$

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 $i = 1, \ldots, n-1$ 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 $i = 1, \ldots, n-1$, nor can it be the case that $b_i = -\hat{c}a_i$ for all $i = 1, \ldots, n-1$. 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 $p_t(\lambda_i)a_ib_i = -\left(\frac{\lambda_{n-1}-\lambda_1}{\lambda_{n-1}+\lambda_1}\right)^t |a_i||b_i|$ for each $i = 1, \ldots, n-1$. 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

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$b_i = \hat{c}a_i \neq 0$, 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 $X = \overline{Y}$. It is straightforward to determine that $\alpha^2 + \beta^2 = \frac{vol(X)vol(\overline{X})}{vol(G)}$ and $\hat{c}^2\alpha^2 + \hat{c}^2\beta^2 = \frac{vol(Y)vol(\overline{Y})}{vol(G)}$, which yields $\hat{c} = \sqrt{\frac{vol(Y)vol(\overline{Y})}{vol(X)vol(\overline{X})}} = c$. □

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

Since X and Y are disjoint, it follows that $d(X,Y)$ is the minimum $k \in I\!N$ such that $< D^{\frac{1}{2}}\psi_Y, \mathcal{L}^k D^{\frac{1}{2}}\psi_X > \neq 0$. For each $k \in I\!N$ we have $< D^{\frac{1}{2}}\psi_Y, \mathcal{L}^k D^{\frac{1}{2}}\psi_X >= -c\alpha^2\lambda_1^k + c\beta^2\lambda_{n-1}^k$. 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, $d(X,Y) \leq 2$.

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 $\sqrt{\frac{vol(\overline{X})vol(\overline{Y})}{vol(X)vol(Y)}} \leq \frac{\lambda_{n-1}+\lambda_1}{\lambda_{n-1}-\lambda_1}$.

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

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

Henceforth we assume that the integer t is equal to $\frac{\log\sqrt{\frac{vol(\overline{X})vol(\overline{Y})}{vol(X)vol(Y)}}}{\log\frac{\lambda_{n-1}+\lambda_1}{\lambda_{n-1}-\lambda_1}}$. 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. □

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