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Stephen J. Kirkland
kirkland@math.uregina.ca

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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 $L$, is given by $L = I - D^{-1/2}AD^{-1/2}$. It turns out that $L$ is a positive semidefinite matrix, having 0 as a simple eigenvalue (see [1]). Denote the eigenvalues of $L$ by $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_{n-1}$. The relationship between the structural properties of $G$ and the eigenvalues of $L$ 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 $\text{vol}(X)$, is defined as the sum of the degrees of the vertices in $X$, while $\text{vol}(G)$ 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 $L$, 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 $X \neq Y, \overline{Y}$. Then we have

$$d(X,Y) \leq \left\lfloor \frac{\log \sqrt{\text{vol}(X)\text{vol}(Y)}}{\log \frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1}} \right\rfloor. \tag{1.1}$$

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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† Department of Mathematics and Statistics, University of Regina, Regina, Saskatchewan, S4S 0A2 Canada (kirkland@math.uregina.ca). Research partially supported by NSERC under grant number OGP0138251.
The normalized Laplacian for \( H(p, q) \) is given by
\[
\begin{bmatrix}
I & \sqrt{\frac{1}{q(p+q-1)}}J \\
-\sqrt{\frac{1}{q(p+q-1)}}J & \frac{p+q}{p+q-1}I - \frac{1}{p+q-1}J
\end{bmatrix}
\]

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 \( \frac{n}{2} \) vertices of degree \( q \), and let \( Y \) denote the set of the remaining \( \frac{n}{2} \) vertices of degree \( q \). Note that \( X \neq \overline{Y} \) and that \( d(X, Y) = 2 \). We have \( \text{vol}(X) = \frac{3p}{2} = \text{vol}(Y) \) and \( \text{vol}(X) = q \left( \frac{3p}{2} + q - 1 \right) = \text{vol}(\overline{Y}) \). Consequently, \( \sqrt{\frac{\text{vol}(X)\text{vol}(Y)}{\text{vol}(X)\text{vol}(\overline{Y})}} = \frac{q}{\sqrt{p+q-1}} = 3 + \frac{2q-2}{p} \). Hence we have
\[
\left\lfloor \frac{\log \frac{\text{vol}(X)\text{vol}(\overline{Y})}{\text{vol}(X)\text{vol}(Y)}}{\log \frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1}} \right\rfloor = 1 < 2 = d(X, Y), \text{ contrary to Assertion 1.1.}
\]

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 \( X \neq Y, \overline{Y} \). Let \( \mathcal{L} = I - D^{-1}AD \) 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 \( \lambda_0 < \lambda_1 \leq \ldots \leq \lambda_{n-1} \), 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 \( \lambda_j \). Let \( \psi_X \) denote the vector of order \( n \) with a 1 in the position corresponding to vertex \( i \) if \( i \in X \) and a 0 otherwise. We define \( \psi_Y \) analogously. Let \( 1 \) 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 \( D^{\frac{1}{2}}\psi_X = a_0v_0 + \sum_{i=1}^{n-1} a_i v_i \) and \( D^{\frac{1}{2}}\psi_Y = b_0v_0 + \sum_{i=1}^{n-1} b_i v_i \). Since \( v_0 = \sqrt{\frac{1}{\text{vol}(G)}}D^{\frac{1}{2}}1 \), 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 \( < D^{\frac{1}{2}}\psi_Y, p_t(\mathcal{L})D^{\frac{1}{2}}\psi_X > \) 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
\[
< D^{\frac{1}{2}}\psi_Y, p_t(\mathcal{L})D^{\frac{1}{2}}\psi_X > = a_0 b_0 + \sum_{i=1}^{n-1} p_t(\lambda_i) a_i b_i
\]
\[
\geq a_0 b_0 - \left( \frac{\lambda_{n-1} - \lambda_1}{\lambda_{n-1} + \lambda_1} \right)^t \sqrt{\sum_{i=1}^{n-1} a_i^2 \sum_{i=1}^{n-1} b_i^2}
\]
\[(2.1)\]
in order to conclude that \( < D^\frac{1}{2} \psi_Y, p_t(L) D^\frac{1}{2} \psi_X > \) is strictly positive.

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

**Theorem 2.1.** Suppose that \( X \neq Y, \tilde{Y} \), and let \( c = \sqrt{\frac{\text{vol}(Y)\text{vol}(\tilde{Y})}{\text{vol}(X)\text{vol}(\tilde{Y})}} \). Suppose that
\[
\sum_{i=1}^{n-1} p_t(\lambda_i) a_i b_i = -\left( \frac{\lambda_{n-1} - \lambda_1}{\lambda_{n-1} + \lambda_1} \right)^t \sum_{i=1}^{n-1} |a_i| |b_i|
\]
and
\[
\sum_{i=1}^{n-1} p_t(\lambda_i) a_i b_i \geq -\left( \frac{\lambda_{n-1} - \lambda_1}{\lambda_{n-1} + \lambda_1} \right)^t \sqrt{\sum_{i=1}^{n-1} a_i^2 \sum_{i=1}^{n-1} b_i^2},
\]
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 \( X \neq Y, \tilde{Y} \), 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
\[
p_t(\lambda_i) a_i b_i = -\left( \frac{\lambda_{n-1} - \lambda_1}{\lambda_{n-1} + \lambda_1} \right)^t |a_i| |b_i| \text{ for each } i = 1, \ldots, n-1.
\]
Hence for each \( i \) such that \( \lambda_i \neq \lambda_1, \lambda_{n-1} \), we have \( a_i = b_i = 0 \). Since
\[
p_t(\lambda_1) = \left( \frac{\lambda_{n-1} - \lambda_1}{\lambda_{n-1} + \lambda_1} \right)^t, \text{ and we find that for each index } i \text{ such that } \lambda_i = \lambda_1, \text{ we must have } b_i = -\hat{c} a_i.
\]
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 \( \lambda_i = \lambda_{i-1} \), we have \( b_i = c a_i \).

Consequently, there is a \( \lambda_1 \)-eigenvector \( w \) of norm 1 and a \( \lambda_{n-1} \)-eigenvector \( u \) of norm 1 and constants \( \alpha, \beta \) such that \( D\lambda X = a_0v_0 + \alpha w + \beta u \) and \( D\lambda Y = b_0v_0 - \epsilon \alpha w + \epsilon \beta u \). Note that \( \alpha \neq 0 \) and \( \beta \neq 0 \), otherwise it follows that either \( X = Y \) or \( X = Y \). It is straightforward to determine that \( \alpha^2 + \beta^2 = \frac{\text{vol}(X)\text{vol}(Y)}{\text{vol}(G)} \) and
\[
\hat{c}^2 \alpha^2 + \hat{c}^2 \beta^2 = \frac{\text{vol}(Y)\text{vol}(Y)}{\text{vol}(G)} ,
\]
which yields \( \hat{c} = \sqrt{\frac{\text{vol}(Y)\text{vol}(Y)}{\text{vol}(X)\text{vol}(X)}} = c . \)

\[ \square \]

**Remark 2.2.** Suppose that \( X \cap Y = \emptyset \), and that (2.2) and (2.3) hold. Since
\[
< D\lambda X , D\lambda Y > = 0 ,
\]
we have \( a_0b_0 - c(\alpha^2 - \beta^2) = 0 \). Substituting our expressions for \( a_0 \) and \( b_0 \) yields \( \alpha^2 - \beta^2 = \frac{\text{vol}(X)\text{vol}(Y)}{\text{vol}(G)} \). As noted in the proof of Theorem 2.1, \( \alpha^2 + \beta^2 = \frac{\text{vol}(X)\text{vol}(X)}{\text{vol}(G)} \), and so we find that \( \alpha^2 = \frac{\text{vol}(X)\text{vol}(X)}{2\text{vol}(G)} \left( 1 + \sqrt{\frac{\text{vol}(Y)\text{vol}(Y)}{\text{vol}(X)\text{vol}(Y)}} \right) \) and \( \beta^2 = \frac{\text{vol}(X)\text{vol}(X)}{2\text{vol}(G)} \left( 1 - \sqrt{\frac{\text{vol}(Y)\text{vol}(Y)}{\text{vol}(X)\text{vol}(Y)}} \right) \). 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
\[
< D\lambda Y , \mathcal{L}^k D\lambda X > 
eq 0 .
\]
For each \( k \in \mathbb{N} \) we have \( < D\lambda Y , \mathcal{L}^k D\lambda X > = -c\alpha^2 \lambda_1^k + c\beta^2 \lambda_{n-1}^k \). 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
\[
\frac{\text{vol}(Y)\text{vol}(Y)}{\text{vol}(X)\text{vol}(Y)} \leq \frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1} .
\]

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

**Proof.** Let \( t = \left[ \log \sqrt{\frac{\text{vol}(X)\text{vol}(Y)}{\text{vol}(G)}} \right] . \) If \( t > \log \sqrt{\frac{\text{vol}(X)\text{vol}(Y)}{\text{vol}(G)}} , \) then it follows from (2.1) that
\[
< D\lambda Y , \mathcal{L}^t D\lambda X > \gg 0 ,
\]
and hence that \( d(X,Y) \leq t \).

Henceforth we assume that the integer \( t \) is equal to \( \left[ \log \sqrt{\frac{\text{vol}(X)\text{vol}(Y)}{\text{vol}(G)}} \right] . \) 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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