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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.

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 $L = I - D^{-1}AD^{-1}$. 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

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

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

Example 1.2. Suppose that $p,q \in \mathbb{N}$, and let $H(p,q) = O_p \lor K_q$, where $O_p$ is the graph on $p$ vertices with no edges, and where $G_1 \lor G_2$ 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

$$
\begin{bmatrix}
I & -\frac{1}{\sqrt{q(p+q-1)}}J \\
-\frac{1}{\sqrt{q(p+q-1)}}J & \rho_{p+q-1}I - \frac{1}{p+q-1}J
\end{bmatrix}.
$$

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 $\frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1} = 3 + 2q - 2p$.

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 $X \neq Y$ and that $d(X, Y) = 2$. We have $\text{vol}(X) = \frac{pa}{2} = \text{vol}(Y)$ and $\text{vol}(X) = \frac{q(3q + q - 1)}{2} = \text{vol}(Y)$. Consequently, $\sqrt{\frac{\text{vol}(X)\text{vol}(Y)}{\text{vol}(X)\text{vol}(Y)}} = \frac{q(3q + q - 1)}{4} = 3 + 2q - 2p$. Hence we have

$$
\left[\log\frac{1}{\log \frac{n_{n-1} + \lambda_1}{n_{n-1} - \lambda_1}}\right] = 1 < 2 = d(X, Y), \text{ contrary to Assertion 1.1.}
$$

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 $X \neq Y, Y$. Let $L = I - D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$ 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 $L$ 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 $L$, 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 there 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 $D^{\frac{1}{2}}\psi_X = a_0v_0 + \sum_{i=1}^{n-1} a_iv_i$ and $D^{\frac{1}{2}}\psi_Y = b_0v_0 + \sum_{i=1}^{n-1} b_iv_i$. Since $v_0 = \frac{1}{\sqrt{\text{vol}(G)}}D^{\frac{1}{2}}1$, 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 $p_t(x) = \left(1 - \frac{2x}{\lambda_{n-1} + \lambda_1}\right)^t$, and for each $t \in \mathbb{N}$, let $p_t(L)$ denote the matrix $(I - \frac{2}{\lambda_{n-1} + \lambda_1}L)^t$. The argument in [1] proceeds via the following approach: if for some $t \in \mathbb{N}$, the inner product $< D^{\frac{1}{2}}\psi_Y, p_t(L)D^{\frac{1}{2}}\psi_X >$ 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

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

(2.1) 

$$
\geq a_0b_0 - \left(\frac{\lambda_{n-1} - \lambda_1}{\lambda_{n-1} + \lambda_1}\right)^t \sum_{i=1}^{n-1} a_i^2 \sum_{i=1}^{n-1} b_i^2
$$
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 the case that \( i = b_i \) for each \( i \) for which our hypothesis implies that equality must hold throughout (2.4). In particular, since \( \alpha, \beta, \) and unit eigenvectors \( w \) and \( \overline{u} \), corresponding to \( \lambda_1 \) and \( \lambda_{n-1} \), respectively, such that

\[
D_i \psi_X = a_0 v_0 + \alpha w + \beta \overline{u}, \quad \text{and}
\]

\[
D_i \psi_Y = b_0 v_0 - \alpha w + c \beta \overline{u}.
\]

Further, \( t \) is odd.

**Proof:** Since

\[
\sum_{i=1}^{n-1} p_i(\lambda) a_i b_i \geq - \left( \frac{\lambda_{n-1} - \lambda_1}{\lambda_{n-1} + \lambda_1} \right)^t \sum_{i=1}^{n-1} |a_i||b_i|
\]

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

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

\[
p_i(\lambda) a_i b_i = - \left( \frac{\lambda_{n-1} - \lambda_1}{\lambda_{n-1} + \lambda_1} \right)^t |a_i||b_i| \text{ for each } i = 1, \ldots, n-1.
\]

Hence for each \( i \) such that \( \lambda_i \neq \lambda_1, \lambda_{n-1} \), we have \( a_i = b_i = 0 \). Since \( p_i(\lambda_1) = \left( \frac{\lambda_{n-1} - \lambda_1}{\lambda_{n-1} + \lambda_1} \right)^t \), we find that for each index \( i \) such that \( \lambda_i = \lambda_1 \), we must have \( b_i = -\hat{c}a_i \). Also, since \( p_i(\lambda_{n-1}) = (-1)^t \left( \frac{\lambda_{n-1} - \lambda_1}{\lambda_{n-1} + \lambda_1} \right)^t \), and since there is at least one index \( i \) such that \( \lambda_i = \lambda_{n-1} \) and...
$b_i = c\alpha_i \neq 0$, we find that $t$ must be odd. It now follows that for every $i$ such that 
$\lambda_i = \lambda_{n-1}$, we have $b_i = c\alpha_i$.

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 $D^2\psi_X = a_0v_0 + \alpha w + \beta u$ and $D^2\psi_Y = 
b_0v_0 + \beta \alpha w + \beta \beta u$. 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 $\alpha^2 + \beta^2 = \frac{\text{vol}(X)\text{vol}(Y)}{\text{vol}(G)}$ and 
$\hat{c}^2 \alpha^2 + \hat{c}^2 \beta^2 = \frac{\text{vol}(Y)\text{vol}(\overline{Y})}{\text{vol}(G)}$, which yields $\hat{c} = \sqrt{\frac{\text{vol}(Y)\text{vol}(\overline{Y})}{\text{vol}(X)\text{vol}(X)}} = c$. □

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

Theorem 2.3. Suppose that $G$ is not a complete graph. Let $X$ and $Y$ be subsets 
of the vertex set of $G$ with $X \neq Y, \overline{Y}$. Then $d(X,Y) \leq \max \left\{ \log \sqrt{\frac{\text{vol}(X)\text{vol}(\overline{Y})}{\text{vol}(X)\text{vol}(Y)}}, 2 \right\}$.

Proof: Let $t = \left\lfloor \log \sqrt{\frac{\text{vol}(X)\text{vol}(\overline{Y})}{\text{vol}(X)\text{vol}(Y)}} \right\rfloor$. If $t > \log \sqrt{\frac{\text{vol}(X)\text{vol}(\overline{Y})}{\text{vol}(X)\text{vol}(Y)}}$, then it follows from (2.1) that 
$< D^2\psi_Y, p_t(\mathcal{L})D^2\psi_X >= 0$, and hence that $d(X,Y) \leq t$.

Henceforth we assume that the integer $t$ is equal to $\log \sqrt{\frac{\text{vol}(X)\text{vol}(\overline{Y})}{\text{vol}(X)\text{vol}(Y)}}$. If strict in-
equality 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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