A new upper bound on the largest normalized Laplacian eigenvalue

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Abstract. Let $G$ be a simple undirected connected graph on $n$ vertices. Suppose that the vertices of $G$ are labelled 1, 2, ..., $n$. Let $d_i$ be the degree of the vertex $i$. The Randić matrix of $G$, denoted by $R$, is the $n \times n$ matrix whose $(i,j)$-entry is $\sqrt{d_i d_j}$ if the vertices $i$ and $j$ are adjacent and 0 otherwise. The normalized Laplacian matrix of $G$ is $\mathcal{L} = I - R$, where $I$ is the $n \times n$ identity matrix. In this paper, by using an upper bound on the maximum modulus of the subdominant Randić eigenvalues of $G$, we obtain an upper bound on the largest eigenvalue of $\mathcal{L}$. We also obtain an upper bound on the largest modulus of the negative Randić eigenvalues and, from this bound, we improve the previous upper bound on the largest eigenvalue of $\mathcal{L}$.

1. Introduction

Let $G = (V, E)$ be a simple undirected graph on $n$ vertices. Some matrices on $G$ are the adjacency matrix $A$, the Laplacian matrix $L = D - A$ and the signless Laplacian matrix $Q = D + L$, where $D$ is the diagonal matrix of vertex degrees. It is well known that $L$ and $Q$ are positive semidefinite matrices and that $(0, 1)$ is an eigenpair of $L$ where $1$ is the all ones vector. Fiedler [16] proved that $G$ is a connected graph if and only if the second smallest eigenvalue of $L$ is positive. This eigenvalue is called the algebraic connectivity of $G$. The signless Laplacian matrix has recently attracted the attention of several researchers. Recent papers on this matrix are [5, 6, 7, 8, 9] and some of its basic properties [6] are:

1. For a connected graph, the smallest eigenvalue of $Q$ is equal to 0 if and only if the graph is bipartite. In this case, 0 is a simple eigenvalue. Then, for a connected graph, the smallest eigenvalue of $Q$ is positive if and only if the graph is not bipartite.

2. If $G$ is a bipartite graph then $Q$ and $L$ have the same characteristic polynomial.


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Other matrices on the graph $G$ are the normalized Laplacian matrix and the Randić matrix of $G$. Suppose that the vertices of $G$ are labelled $1, 2, \ldots, n$. Let $d_i$ be the degree of the vertex $i$. Let $D^{-\frac{1}{2}}$ be the diagonal matrix whose diagonal entries are

$$\frac{1}{\sqrt{d_1}}, \frac{1}{\sqrt{d_2}}, \ldots, \frac{1}{\sqrt{d_n}}$$

whenever $d_i \neq 0$. If $d_i = 0$ for some $i$ then the corresponding diagonal entry of $D^{-\frac{1}{2}}$ is defined to be 0. The normalized Laplacian matrix of $G$, denoted by $\mathcal{L}$, was introduced by F. Chung [15] as

$$\mathcal{L} = D^{-\frac{1}{2}}LD^{-\frac{1}{2}} = I - D^{-\frac{1}{2}}AD^{-\frac{1}{2}}. \quad (1)$$

The eigenvalues of $\mathcal{L}$ are called the normalized Laplacian eigenvalues of $G$. From (1), we have

$$D^{\frac{1}{2}} \mathcal{L} D^{\frac{1}{2}} = D - A = L$$

and thus

$$D^{\frac{1}{2}} \mathcal{L} D^{\frac{1}{2}} 1 = L 1 = 01.$$

Hence 0 is an eigenvalue of $\mathcal{L}$ with eigenvector $D^{\frac{1}{2}} 1$.

We recall the following results on $\mathcal{L}$ [15] :

1. The eigenvalues of $\mathcal{L}$ lie in the interval $[0, 2]$.
2. 0 is a simple eigenvalue of $\mathcal{L}$ if and only if $G$ is connected.
3. 2 is an eigenvalue of $\mathcal{L}$ if and only if a connected component of $G$ is bipartite and nontrivial.

Among papers on $\mathcal{L}$, we mention [10, 11, 13, 14] and [17].

From now on, we assume that $G$ is connected graph. Then $d_i > 0$ for all $i$. The notation $i \sim j$ means that the vertices $i$ and $j$ are adjacent. The matrix $R = D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$ in (1) is the Randić matrix of $G$ in which the $(i, j)$-entry is $\frac{1}{\sqrt{d_i d_j}}$ if $i \sim j$ and 0 otherwise. Moreover

$$I - \mathcal{L} = R.$$

The eigenvalues of $R$ are called the Randić eigenvalues of $G$. Clearly $\mathcal{L}$ and $R$ are both real symmetric matrices. The Randić matrix was earlier studied in connection with the Randić index [1, 2, 18] and [19]. Two recent papers on the Randić matrix are [3] and [4].

Throughout this paper

$$0 = \lambda_n \leq \lambda_{n-1} \leq \ldots \leq \lambda_1$$

and

$$\rho_n \leq \rho_{n-1} \leq \ldots \leq \rho_1.$$
are the normalized Laplacian eigenvalues and the Randić eigenvalues of \( \mathcal{G} \), respectively. It follows that
\[
\lambda_i = 1 - \rho_{n-i+1} \quad (1 \leq i \leq n).
\]

If \( M \) is a nonnegative matrix then, by the Perron-Frobenius Theorem, \( M \) has an eigenvalue equal to its spectral radius, called the Perron root of \( M \). In addition, if \( M \) is irreducible then the Perron root of \( M \) is a simple eigenvalue with a corresponding positive eigenvector, called the Perron vector of \( M \). Since \( \mathcal{G} \) is a connected graph, Randić matrix of \( \mathcal{G} \) is an irreducible nonnegative matrix. Let \( \mathbf{v} = D^{\frac{1}{2}} \mathbf{1} \). Then
\[
\mathbf{v} = \begin{bmatrix} \sqrt{d_1}, \sqrt{d_2}, \ldots, \sqrt{d_n} \end{bmatrix}^T.
\]

An easy computation shows that
\[
R\mathbf{v} = \mathbf{v}.
\]

Hence, 1 and \( \mathbf{v} \) are the Perron root and the Perron vector of \( R \), respectively.

Let \( \Delta \) and \( \delta \) be the largest and smallest vertex degrees of \( \mathcal{G} \), respectively, and let \( q_n \) be the smallest eigenvalue of \( Q \).

A recent result involving the largest eigenvalue of \( L \) and the smallest eigenvalue of \( Q \) is

**THEOREM 1.** [17] Let \( \mathcal{G} \) be a connected graph. Then
\[
2 - \frac{q_n}{\delta} \leq \lambda_1 \leq 2 - \frac{q_n}{\Delta}. \tag{2}
\]

We may consider \( 2 - \frac{q_n}{\Delta} \) as an upper bound on \( \lambda_1 \). Observe that \( 2 - \frac{q_n}{\Delta} = 2 \) if and only if \( \mathcal{G} \) is a bipartite graph.

In this paper, we search for a new upper bound on \( \lambda_1 \) not exceeding the trivial upper bound 2.

2. Searching for an upper bound on \( \lambda_1 \)

Since \( \sum_{i=1}^{n} \rho_i = tr(R) = 0 \), it follows that \( \rho_n < 0 \). We have
\[
\lambda_1 = 1 - \rho_n = 1 + |\rho_n|.
\]

In order to find an upper bound on \( \lambda_1 \) not exceeding 2, we look for an upper bound on \( |\rho_n| \) not exceeding 1.

An eigenvalue of a nonnegative matrix \( M \) which is different from the Perron root is called a subdominant eigenvalue of \( M \). Let \( \xi(M) \) be the maximum modulus of the subdominant eigenvalues of \( M \). Special attention has been devoted to find upper bounds on \( \xi(M) \). In [20], we can find a unified presentation of results concerning upper bounds on \( \xi(M) \). These upper bounds are important because \( \xi(M) \) plays a major role in convergence properties of powers of \( M \). Since
\[
\lambda_1 \leq 1 + \xi(R), \tag{3}
\]
we focus our attention on upper bounds on \( \xi(R) \). We recall the result [12, p. 295]:
THEOREM 2. If \( M = (m_{i,j}) \geq 0 \) of order \( n \times n \) has a positive eigenvector \( w = [w_1, w_2, \ldots, w_n]^T \) corresponding to the spectral radius \( \rho(M) \) of \( M \) then
\[
\xi(M) \leq \frac{1}{2} \max_{i<j} \sum_{k=1}^{n} w_k \left| \frac{m_{i,k}}{w_i} - \frac{m_{j,k}}{w_j} \right|.
\]
where the maximum is taken over all pairs \((i, j)\), \(1 \leq i < j \leq n\).

In order to apply Theorem 2, it is convenient to observe that the Randić matrix of \( G \) is diagonally similar to the row stochastic matrix
\[
S = D^{-\frac{1}{2}}RD^{\frac{1}{2}}.
\]
(4)

The following lemma gives some immediate properties of \( S \).

LEMA 1. 1. The \((i, j)\)–entry of \( S \) is \( \frac{1}{d_i} \) if \( j \sim i \) and \( 0 \) otherwise.
2. \( S1 = 1 \) where \( 1 \) is the all ones vector.
3. \( u \) is an eigenvector for \( R \) corresponding to the eigenvalue \( \alpha \) if and only if \( D^{-\frac{1}{2}}u \) is an eigenvector for \( S \) corresponding to the eigenvalue \( \alpha \).
4. If \( G \) is an \( r \)–regular graph then \( S = R \).

Let \( N_i \) be the set of neighbours of the vertex \( v_i \) and let \( |N_i| \) be the cardinality of \( N_i \).

THEOREM 3. Let \( G \) be a simple undirected connected graph. If \( \lambda_1 \) is the largest eigenvalue of \( L \) then
\[
|\lambda_1| \leq 2 - \min_{i<j} \left\{ \frac{|N_i \cap N_j|}{\max\{d_i, d_j\}} \right\}
\]
where the minimum is taken over all pairs \((i, j)\), \(1 \leq i < j \leq n\).

Proof. We know that the Randić matrix of \( G \) is similar to the row stochastic matrix \( S \) defined in (4). Then \( \xi(R) = \xi(S) \). The eigenvector corresponding to the spectral of \( S \) is \( w = 1 \). Applying Theorem 2 to \( S = (s_{i,j}) \), we have
\[
\xi(S) \leq \frac{1}{2} \max_{i<j} \sum_{k=1}^{n} |s_{i,k} - s_{j,k}|
= \frac{1}{2} \max_{i<j} \left( \sum_{k \in N_i - N_j} \frac{1}{d_i} + \sum_{k \in N_j - N_i} \frac{1}{d_j} + \sum_{k \in N_i \cap N_j} \left| \frac{1}{d_i} - \frac{1}{d_j} \right| \right)
= \frac{1}{2} \max_{i<j} \left( \frac{|N_i - N_j|}{d_i} + \frac{|N_j - N_i|}{d_j} + \sum_{k \in N_i \cap N_j} \left| \frac{1}{d_i} - \frac{1}{d_j} \right| \right)
= \frac{1}{2} \max_{i<j} \left( 2 - \frac{|N_i \cap N_j|}{d_i} - \frac{|N_j \cap N_i|}{d_j} + \sum_{k \in N_i \cap N_j} \left| \frac{1}{d_i} - \frac{1}{d_j} \right| \right).
\]
Suppose \( d_i = \max \{d_i, d_j\} \). In this case
\[
2 - \frac{|N_i \cap N_j|}{d_i} - \frac{|N_j \cap N_i|}{d_j} + \sum_{k \in N_i \cap N_j} \left| \frac{1}{d_i} - \frac{1}{d_j} \right|
= 2 - \frac{|N_i \cap N_j|}{d_i} - \frac{|N_j \cap N_i|}{d_j} + \left( \frac{1}{d_j} - \frac{1}{d_i} \right) |N_i \cap N_j|
= 2 - 2 \frac{|N_i \cap N_j|}{d_i}.
\]

Similarly, if \( d_j = \max \{d_i, d_j\} \) then
\[
2 - \frac{|N_i \cap N_j|}{d_i} - \frac{|N_j \cap N_i|}{d_j} + \sum_{k \in N_i \cap N_j} \left| \frac{1}{d_i} - \frac{1}{d_j} \right|
= 2 - 2 \frac{|N_j \cap N_i|}{d_j}.
\]

Hence
\[
\xi(S) \leq \frac{1}{2} \max_{i < j} \sum_{k=1}^{n} \left| s_{i,k} - s_{j,k} \right|
= \frac{1}{2} \max_{i < j} \left\{ 2 - 2 \frac{|N_j \cap N_i|}{\max \{d_i, d_j\}} \right\}
= 1 - \min_{i < j} \left\{ \frac{|N_i \cap N_j|}{\max \{d_i, d_j\}} \right\}
\]

Since \( \lambda_1 \leq 1 + \xi(R) = 1 + \xi(S) \), the upper bound in (5) follows. □

**Remark 1.** If \( G \) is a bipartite graph then \( |N_i \cap N_j| = 0 \), for some \( i < j \), and consequently the upper bound in (5) is equal to 2. This is sufficient condition but it is not a necessary condition. In fact, there are other instances in which \( N_i \cap N_j = 0 \) for some \( i < j \). One of them is given by a nonbipartite graph having a bridge. However, if \( \min_{i < j} |N_i \cap N_j| \geq 1 \) and \( q_n < 1 \) then
\[
2 - \min_{i < j} \left\{ \frac{|N_i \cap N_j|}{\max \{d_i, d_j\}} \right\} < 2 - \frac{q_n}{\Delta}. \tag{6}
\]

In fact
\[
q_n < 1 \leq |N_i \cap N_j| \text{ for } i < j
\]
and
\[
\frac{q_n}{\Delta} \leq \frac{1}{\max \{d_i, d_j\}} \text{ for } i < j.
\]
Then
\[ \frac{q_n}{\Delta} < \frac{|N_i \cap N_j|}{\max \{d_i, d_j\}} \quad \text{for } i < j. \]

It follows
\[ 2 - \frac{q_n}{\Delta} > 2 - \min_{i < j} \frac{|N_i \cap N_j|}{\max \{d_i, d_j\}}. \]

Hence, if \( \min_{i < j} |N_i \cap N_j| \geq 1 \) and \( q_n < 1 \) then (5) gives a better upper bound for \( \lambda_1 \) than the second inequality in (2) does.

3. Improving the upper bound on \( \lambda_1 \)

We have
\[ \lambda_1 = u1 + |q_n| \leq 1 + \xi (R) = 1 + \xi (S). \]

The upper bound on \( \lambda_1 \) in (5) was obtained by using an upper bound on \( \xi (R) \). In this section, in order to get an improved upper bound on \( \lambda_1 \), we search for an upper bound on \( |q_n| \), that is, on the largest modulus of the negative Randić eigenvalues.

**Theorem 4.** Let \( G \) be a simple undirected connected graph. If \( \rho_n \) is eigenvalue with the largest modulus among the negative Randić eigenvalues of \( G \) then
\[ |\rho_n| \leq 1 - \min_{i \sim j} \left\{ \frac{|N_i \cap N_j|}{\max \{d_i, d_j\}} \right\}, \]
where the minimum is taken over all pairs \((i, j)\), \(1 \leq i < j \leq n\), such that the vertices \( i \) and \( j \) are adjacent.

**Proof.** Let \( \rho_n \) be the largest modulus of the negative Randić eigenvalues of \( G \). Let
\[ \mathbf{x} = [x_1, x_2, \ldots, x_n]^T \]
be such that
\[ S\mathbf{x} = \rho_n \mathbf{x}. \quad (7) \]
From Lemma 1, we have \( \mathbf{x} = D^{-\frac{1}{2}} \mathbf{u} \) where \( R\mathbf{u} = \rho_n \mathbf{u} \). Since \( \mathbf{u} \) is orthogonal to the Perron vector \( \mathbf{v} = [\sqrt{d_1}, \sqrt{d_2}, \ldots, \sqrt{d_n}]^T \), the vector \( \mathbf{u} \) has at least one positive component and at least one negative component. Since \( \mathbf{x} = D^{-\frac{1}{2}} \mathbf{u} \), this is also true for the vector \( \mathbf{x} \). Let
\[ \max \{x_1, x_2, \ldots, x_n\} = x_i \]
and let
\[ x_j = \min \{x_k : k \sim i\}. \]
Since \( \mathbf{x} \) has at least one positive component, \( x_i > 0 \). Let \( S = (s_{i,j}) \). From (7)
\[ \rho_n x_j = \sum_{k=1}^{n} s_{j,k} x_k = \frac{1}{d_j} \sum_{k \in N_j} x_k \quad (8) \]
and

$$\rho_n x_i = \sum_{k=1}^{n} s_{i,k} x_k = \frac{1}{d_i} \sum_{k \in N_i} x_k. \quad (9)$$

Subtracting (9) from (8), we get

$$\rho_n (x_j - x_i) = \frac{1}{d_j} \sum_{k \in N_j} x_k - \frac{1}{d_i} \sum_{k \sim i} x_k. \quad (10)$$

Then

$$q_n (x_j - x_i) = \frac{1}{d_j} \sum_{k \in N_j - N_i} x_k + \frac{1}{d_j} \sum_{k \in N_j \cap N_i} x_k - \frac{1}{d_i} \sum_{k \in N_i - N_j} x_k - \frac{1}{d_i} \sum_{k \in N_i \cap N_j} x_k. \quad (10)$$

By definition, $x_j \leq x_k$ for all $k \sim i$ and $x_k \leq x_i$ for all $k$. Hence

$$\sum_{k \in N_j - N_i} x_k \leq |N_j - N_i| x_i \quad (11)$$

and

$$- \sum_{k \in N_i - N_j} x_k \leq - |N_i - N_j| x_j. \quad (12)$$

Replacing the inequalities (11) and (12) in (10), we obtain

$$q_n (x_j - x_i) \leq \frac{1}{d_j} |N_j - N_i| x_i - \frac{1}{d_i} |N_i - N_j| x_j + \sum_{k \in N_j \cap N_i} \left( \frac{1}{d_j} - \frac{1}{d_i} \right) x_k.$$

Thus

$$q_n (x_j - x_i) \leq \frac{1}{2} \frac{1}{d_j} |N_j - N_i| (x_i - x_j) + \frac{1}{2} \frac{1}{d_i} |N_i - N_j| (x_i - x_j)$$

$$+ \frac{1}{2} \left( \frac{1}{d_j} |N_j - N_i| - \frac{1}{d_i} |N_i - N_j| \right) (x_i + x_j)$$

$$+ \sum_{k \in N_j \cap N_i} \left( \frac{1}{d_j} - \frac{1}{d_i} \right) x_k.$$

Clearly

$$\frac{1}{d_j} |N_j - N_i| - \frac{1}{d_i} |N_i - N_j| = \left( \frac{1}{d_i} - \frac{1}{d_j} \right) |N_i \cap N_j|. $$
Hence
\[
\rho_n(x_j - x_i) \leq \frac{1}{2} \left( \frac{1}{d_j} |N_j - N_i| (x_i - x_j) + \frac{1}{2} d_i |N_i - N_j| (x_i - x_j) \right)
+ \frac{1}{2} \left( \frac{1}{d_j} - \frac{1}{d_i} \right) |N_i \cap N_j| (x_i + x_j) + \frac{1}{2} \sum_{k \in N_i \cap N_j} \left( \frac{1}{d_j} - \frac{1}{d_i} \right) (x_k + x_k)
= \frac{1}{2} \left( \frac{1}{d_j} |N_j - N_i| (x_i - x_j) + \frac{1}{2} d_i |N_i - N_j| (x_i - x_j) \right)
+ \frac{1}{2} \sum_{k \in N_i \cap N_j} \left( \frac{1}{d_j} - \frac{1}{d_i} \right) (x_i - x_k + x_j - x_k).
\]
Moreover
\[
\sum_{k \in N_i \cap N_j} \left( \frac{1}{d_i} - \frac{1}{d_j} \right) (x_i - x_k + x_j - x_k)
\leq \sum_{k \in N_i \cap N_j} \left( \frac{1}{d_i} - \frac{1}{d_j} \right) (x_i - x_k) + \sum_{k \in N_i \cap N_j} \left( \frac{1}{d_i} - \frac{1}{d_j} \right) (x_k - x_j)
= \sum_{k \in N_i \cap N_j} \left( \frac{1}{d_i} - \frac{1}{d_j} \right) (x_i - x_j).
\]
Therefore
\[
\rho_n(x_j - x_i) \leq \frac{1}{2} \left( \frac{1}{d_j} |N_j - N_i| (x_i - x_j) + \frac{1}{2} d_i |N_i - N_j| (x_i - x_j) \right)
+ \frac{1}{2} \sum_{k \in N_i \cap N_j} \left( \frac{1}{d_i} - \frac{1}{d_j} \right) (x_i - x_j).
\]
If \(x_j = x_i\) then \(x_k = x_i\) for all \(k \sim i\). Consequently, from \(Sx = \rho_n x\), we have
\[
q_n x_i = \sum_{k \in N_i} \frac{1}{d_i} x_k = \frac{1}{d_i} \sum_{k \in N_i} x_i = \frac{x_i}{d_i} d_i = x_i.
\]
Thus \(\rho_n = 1\), which is a contradiction. Hence \(x_i - x_j > 0\). Dividing both sides of (13) by \((x_i - x_j)\), we obtain
\[
-\rho_n \leq \frac{1}{2} \left( \frac{1}{d_j} |N_j - N_i| + \frac{1}{2} d_i |N_i - N_j| + \frac{1}{2} \sum_{k \in N_i \cap N_j} \left( \frac{1}{d_i} - \frac{1}{d_j} \right) \right).
\]
As in the proof of Theorem 3, we get
\[
\frac{1}{2} \frac{1}{d_j} |N_j - N_i| + \frac{1}{2} \frac{1}{d_i} |N_i - N_j| + \frac{1}{2} \sum_{k \in N_i \cap N_j} \left( \frac{1}{d_i} - \frac{1}{d_j} \right)
= 1 - \frac{|N_i \cap N_j|}{\max \{d_i, d_j\}}.
\]
Consequently

\[ |\rho_n| \leq 1 - \frac{|N_i \cap N_j|}{\max \{d_i, d_j\}}. \]

Observe that the vertices \( v_i \) and \( v_j \) are adjacent. Hence

\[ |\rho_n| \leq \max_{i \sim j} \left\{ 1 - \frac{|N_i \cap N_j|}{\max \{d_i, d_j\}} \right\} = 1 - \min_{i \sim j} \left\{ \frac{|N_i \cap N_j|}{\max \{d_i, d_j\}} \right\}. \]

The proof is complete. \( \square \)

Finally, we have

**Theorem 5.** Let \( \mathcal{G} \) be a simple undirected connected graph. If \( \lambda_1 \) is the largest normalized Laplacian eigenvalue of \( \mathcal{G} \) then

\[ \lambda_1 \leq 2 - \min_{i \sim j} \left\{ \frac{|N_i \cap N_j|}{\max \{d_i, d_j\}} \right\} \]

where the minimum is taken over all pairs \((i, j)\), \(1 \leq i < j \leq n\), such that the vertices \(i\) and \(j\) are adjacent.

**Proof.** Since \( \lambda_1 = 1 - \rho_n = 1 + |\rho_n| \), the proof is immediate using the upper bound on \( |\rho_n| \) given by Theorem 4. \( \square \)

**Example 1.** \( \mathcal{G} \):

Let

\[ b(i, j) = \frac{|N_i \cap N_j|}{\max \{d_i, d_j\}} \]

For this graph

\[ b(1, 2) = \frac{1}{2}, \quad b(1, 3) = b(2, 3) = b(3, 4) = b(3, 5) = \frac{1}{5}, \quad b(3, 6) = \frac{2}{5}, \quad b(4, 6) = b(5, 6) = \frac{1}{3}. \]

Then \( \min_{i \sim j} b(i, j) = \frac{1}{5} \). Hence the largest modulus of the negative Randić eigenvalues is bounded above by \( \frac{4}{5} \) and the largest normalized Laplacian eigenvalue is bounded above by \( \frac{9}{5} = 1.8 \). To four decimal places the smallest signless Laplacian eigenvalue of \( \mathcal{G} \) is 0.7411. Since \( \Delta = 5 \), the upper bound in (2) becomes \( 2 - \frac{0.7411}{5} = 1.8518 \).
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