On the sum of signless Laplacian eigenvalues of a graph

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Abstract

For a simple graph G, let $e(G)$ denote the number of edges and $S_k(G)$ denote the sum of the k largest eigenvalues of the signless Laplacian matrix of G. We conjecture that for any graph G with n vertices, $S_k(G) \leq e(G) + \binom{k+1}{2}$ for $k = 1, \ldots, n$. We prove the conjecture for $k = 2$ for any graph, and for all k for regular graphs. The conjecture is an analogous to a conjecture by A.E. Brouwer with a similar statement but for the eigenvalues of Laplacian matrices of graphs.

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1 Introduction

Let G be a simple graph with vertex set $V(G) = \{v_1, \ldots, v_n\}$. The degree of a vertex $v \in V(G)$, denoted by $d(v)$, is the number of neighbors of v. The *adjacency matrix* of G is an $n \times n$ matrix $A(G)$ whose (i, j) entry is 1 if v_i and v_j are adjacent and zero otherwise. The *Laplacian matrix* and the *signless Laplacian matrix* of G are the matrices $L(G) = A(G) - D(G)$ and $Q(G) = A(G) + D(G)$, respectively, where $D(G)$ is the diagonal matrix with $d(v_1), \ldots, d(v_n)$ on its main diagonal. It is well-known that $L(G)$ and $Q(G)$ are positive semidefinite and so their eigenvalues are nonnegative real numbers. The eigenvalues of $L(G)$ and $Q(G)$ are called the *Laplacian eigenvalues* and *signless Laplacian eigenvalues* of G, respectively, and are denoted by $\mu_1(G) \geq \cdots \geq \mu_n(G)$ and $q_1(G) \geq \cdots \geq q_n(G)$, respectively. We drop G from the notation when there is no danger of confusion. Note that each row sum of $L(G)$ is 0 and therefore, $\mu_n(G) = 0$. We denote the edge set of G by $E(G)$ and we let $e(G) = |E(G)|$.

Grone and Merris [9] conjectured that for a graph G with degree sequence $d_1, \dots, d_n$, the following holds:

$$\sum_{i=1}^{k} \mu_i(G) \le \sum_{i=1}^{k} \#\{\ell \mid d_\ell \ge i\}, \quad \text{for } k = 1, \dots, n. \tag{1}$$

This conjecture was recently proved by Hua Bai [1]. As a variation on the Grone-Merris conjecture, Brouwer [3, p. 53] conjectured that for a graph G with n vertices,

$$\sum_{i=1}^{k} \mu_i(G) \le e(G) + \binom{k+1}{2}, \quad \text{for } k = 1, \dots, n.$$

The conjecture is known to be true for

(i) $k = n$ and $k = n - 1$ (straightforward);

(ii) $k = 1$ by the well-known inequality $\mu_1(G) \le n$;

(iii) $k = 2$ [10];

(iv) trees [10];

(v) unicyclic and bicyclic graphs [5] (see also [15]);

(vi) regular graphs [2, 11];

(vii) split graphs (graphs whose vertex set can be partitioned into a clique and an independent set) [2, 11];

(viii) cographs (graphs with no path on 4 vertices as an induced subgraph) [2, 11];

(ix) graphs with at most 10 vertices [2, 11].

We remark that (iv) was proved in [10] by showing that $\sum_{i=1}^{k} \mu_i(T) \le e(G) + 2k - 1$ for any tree T. This was improved in [8] to the stronger inequality $\sum_{i=1}^{k} \mu_i(T) \le e(T) + 2k - 1 - \frac{2k-2}{n}$.

For a graph G, let

$$S_k(G) := \sum_{i=1}^{k} q_i(G).$$

In analogy to Brouwer's conjecture, we put forward the following.

Conjecture 1. *For any graph G with n vertices and any $k = 1, \dots, n$,*

$$S_k(G) \le e(G) + \binom{k+1}{2}. \tag{2}$$

To support Conjecture 1, we prove that it holds for $k = 1, 2$ for any graph, and for all k for regular graphs. By computation we establish Conjecture 1 for all graphs up to 10 vertices. Similar to Brouwer's conjecture, Conjecture 1 is straightforward for $k = n$ and $k = n-1$. As it is well-known that $Q(G)$ and $L(G)$ are similar if G is bipartite (see [4, p. 217]), the correctness of Conjecture 1 for trees follows from that of Brouwer's conjecture. We also show that Conjecture 1 is asymptotically tight for any k.

2 Preliminaries

For a subset X of $V(G)$, $N(X)$ denotes the set of vertices outside X, which have at least one neighbor in X. An *independent set* in G is a subset Y of $V(G)$ such that no two distinct vertices in Y are adjacent. A set of edges which pairwise have no common endpoints is called a *matching.* The maximum size of a matching in G is called the *matching number* of G, denoted by $m(G)$. For two graphs G_1 and G_2, *the union* of G_1 and G_2, denoted by $G_1 \cup G_2$, is the graph whose vertex set is $V(G_1) \cup V(G_2)$ and whose edge set is $E(G_1) \cup E(G_2)$. The complement of G is denoted by $\bar{G}$. We denote the complete graph, star and path with n vertices by K_n, S_n and P_n, respectively. The complete bipartite graph with the part sizes m and n is denoted by $K_{m,n}$. First, we recall the following two well known result.

Theorem 2. (see [4, p. 222]) *Let G be a graph with n vertices and let G' be a graph obtained from G by inserting a new edge into G. Then the signless Laplacian eigenvalues of G and G' interlace, that is,*

$$q_1(G') \geq q_1(G) \geq q_2(G') \geq q_2(G) \geq \cdots \geq q_n(G') \geq q_n(G).$$

Theorem 3. ([6]) *Let A and B be two Hermitian matrices of size n. Then for any $1 \leq k \leq n$,*

$$\sum_{i=1}^{k} \lambda_i(A+B) \leq \sum_{i=1}^{k} \lambda_i(A) + \sum_{i=1}^{k} \lambda_i(B),$$

where $\lambda_1(X) \geq \cdots \geq \lambda_n(X)$ denote the eigenvalues of Hermitian matrix X.

The following is straightforward.

Lemma 4. *If for some k, (2) holds for G and H, then it does for $G \cup H$.*

Therefore, in order to prove (2) for some k, it suffices to do so for connected graphs.

Theorem 5. *Conjecture 1 is true for $k = 1, n-1, n$.*

Proof. By Lemma 4, it suffices to consider connected graphs. The result for $k = 1$ follows from the fact that $e(G) \geq n - 1$ as well as the inequality $q_1(G) \leq \frac{2e(G)}{n-1} + n - 2$, for any graph G ([7]). So we have $q_1(G) \leq e(G) + 1$.

For $k = n - 1, n$, (2) follows as $S_{n-1}(G) \leq S_n(G) = 2e(G) \leq e(G) + \binom{n}{2}$. $\square$

Using the McKay's database on small graphs [12], by a computer search we checked Conjecture 1 for graphs with at most 10 vertices.

Lemma 6. *Conjecture* 1 *is true for all graphs on at most* 10 *vertices.*

Lemma 7. *Let* n *be a positive integer.*

(i) *The signless Laplacian eigenvalues of* K_n *are* $2n-2$ *and* $n-2$ *with multiplicities* 1 *and* $n-1$, *respectively.*

(ii) *The signless Laplacian eigenvalues of* S_n *are* n, 1 *and* 0 *with multiplicities* 1, $n-2$, *and* 1, *respectively.*

We close this section by a remark on tightness of (2).

Remark 8. We show that for any k, the conjectured inequality (2) is asymptotically tight. Let $G = G(k,t)$ denote the graph $K_k \vee \overline{K_t}$, the join of K_k and the empty graph $\overline{K_t}$. We have

$$e(G) + \binom{k+1}{2} = tk + \binom{k}{2} + \binom{k+1}{2} = k(t+k).$$

The graph G has an obvious equitable partition where the corresponding quotient matrix of $Q = Q(G)$ is

$$\begin{pmatrix} 2k+t-2 & t \\ k & k \end{pmatrix},$$

with characteristic polynomial

$$f(x) := x^2 + (2 - t - 3k)x + 2k^2 - 2k.$$

On the other hand, $Q - (k+t-2)I$ and $Q - kI$ have k and t identical rows, respectively, thus Q has eigenvalues $k+t-2$ and k with multiplicities at least $k-1$ and $t-1$, respectively. It follows that the characteristic polynomial of Q is

$$(x - k - t + 2)^{k-1}(x - k)^{t-1} f(x).$$

Now, by virtue of

$$f(3k + t - 2) = 2k^2 - 2k, \quad \text{and} \quad f\left(3k + t - 2 - \frac{1}{\sqrt{t}}\right) = -\sqrt{t} + 2k^2 - 2k + \frac{2 - 3k}{\sqrt{t}} + \frac{1}{t},$$

we see that, with t sufficiently large, $3k+t-2-1/\sqrt{t} < q_1(G) \le 3k+t-2$. It turns out that

$$\begin{aligned} S_k(G) &> (k-1)(k+t-2) + 3k + t - 2 - \frac{1}{\sqrt{t}} \\ &= k(k+t) - \frac{1}{\sqrt{t}}, \end{aligned}$$

for large enough t. This shows that the inequality (2) is asymptotically tight for any k.

3 Regular graphs

In this section, we prove that Conjecture 1 holds for regular graphs. We start with the following lemma.

Lemma 9. *Let G be an r-regular graph on n vertices. If either*

(i) $4kr + n^2 + n \le 2nr + 2kn + 2k$, *or*

(ii) $4kr + 2n^2 \le 3nr + 2kn + k^2 + k$,

then $S_k(G) \le e(G) + \binom{k+1}{2}$.

Proof. We have $q_i = 2r - \mu_{n-i+1}$ for $i = 1, \dots, n$. Since Brouwer's conjecture holds for regular graphs ([2, 11]), we have

$$\begin{aligned} \sum_{i=1}^{k} q_i &= 2kr - 2e + \sum_{i=1}^{n-k} \mu_i \\ &\le 2kr - 2e + e + \binom{n-k+1}{2}. \end{aligned}$$

If (i) holds, then $2kr - 2e + e + \binom{n-k+1}{2} \le e + \binom{k+1}{2}$ and we are done. On the other hand, since $\mu_1 \le n$ we have $\sum_{i=1}^{n-k} \mu_i \le n(n-k)$ and similarly if (ii) holds, we yield the result. □

Lemma 10. *Let G be an r-regular graph on n vertices and suppose that $4k \le n + 2r + 3$. If $S_k(G) \le e(G) + \binom{k+1}{2}$, then $S_{n-k+1}(\overline{G}) \le e(\overline{G}) + \binom{n-k+1}{2}$.*

Proof. Let $\overline{q}_1 \ge \cdots \ge \overline{q}_n$ be the signless Laplacian eigenvalues of $\overline{G}$. Then $\overline{q}_1 = 2(n-r-1)$ and

$\overline{q}_i = n-2-q_{n-i+2}$ for $i=2,\dots,n$. So we have

$$\begin{aligned}\sum_{i=1}^{n-k+1} \overline{q}_i &= 2(n-r-1)+(n-k)(n-2)-\sum_{i=k+1}^{n} q_i \\ &= 2(n-r-1)+(n-k)(n-2)-2e(G)+\sum_{i=1}^{k} q_i \\ &\le 2(n-r-1)+(n-k)(n-2)-\binom{n}{2}+e(\overline{G})+\binom{k+1}{2} \\ &\le e(\overline{G})+\binom{n-k+2}{2}.\end{aligned}$$

The last inequality follows from $4k \le n+2r+3$. □

Lemma 11. ([13, 14]) *Let A be a $(0,1)$-symmetric matrix with eigenvalues $\theta_1 \ge \cdots \ge \theta_n$, then*

$$\theta_1+\cdots+\theta_k \le \frac{n}{2}\left(1+\sqrt{k}\right), \quad \textit{for } k=1,\dots,n.$$

If G is an r-regular graph, then $Q(G)=(r-1)I+(A(G)+I)$. If $\theta_1 \ge \cdots \ge \theta_n$ are eigenvalues of $A(G)+I$, then by Lemma 11,

$$q_1+\cdots+q_k = k(r-1)+\theta_1+\cdots+\theta_k \le k(r-1)+\frac{n}{2}\left(1+\sqrt{k}\right). \tag{3}$$

Theorem 12. *Conjecture* 1 *holds for regular graphs.*

Proof. Let the adjacency eigenvalues of r-regular graph G be $\theta_1 \ge \cdots \ge \theta_n$. Then $q_i = r+\theta_i$ for $i=1,\dots,n$. Using the Cauchy-Schwarz inequality and the fact that $\sum_{i=1}^n \theta_i^2 = 2e = nr$, we observe that

$$\sum_{i=1}^{k} q_i = kr+\sum_{i=1}^{k}\theta_i \le kr+\left(k\sum_{i=1}^{k}\theta_i^2\right)^{\frac{1}{2}} \le kr+\sqrt{knr}.$$

If we show that the right hand side is at most $\frac{nr}{2}+\binom{k+1}{2}$, then the proof is complete. So it suffices to show that

$$nr+k^2+k-2kr-2\sqrt{nkr} \ge 0.$$

The left hand side is a quadratic function in $\sqrt{r}$. Substituting $\sqrt{r}=x$ we may write it as

$$\begin{aligned} f(x) &= (n-2k)x^2-2\sqrt{nk}x+k^2+k \\ &= (n-2k)\left(x-\frac{\sqrt{nk}}{n-2k}\right)^2+k^2+k-\frac{nk}{n-2k}. \end{aligned} \tag{4}$$

Now we consider three cases.

Case 1. $n \geq 2k + 2$.

In this case, (4) is nonnegative, as desired.

Case 2. $n = 2k + 1$.

If $r \geq n/2$, then the result follows from Lemma 9 (i). Suppose that $r < \frac{n}{2}$. The roots of $f(x)$ are $\sqrt{n(n-1)/2} \pm (n-1)/2$. Both the roots are greater than $\sqrt{n/2}$ for $n \geq 11$. So for $n \geq 11$, we have $f(\sqrt{r}) > 0$, as desired. Since in this case n is odd, the assertion for the remaining values of n follows from Lemma 6.

Case 3. $n \leq 2k$.

The result for $k \geq 3n/4$ follows in view of Lemma 10 and the fact that the theorem is true for $k \leq n/4$ by Case 2. So we only need to prove the theorem for $n/2 \leq k < 3n/4$. First assume that $r \leq 3n/4$. By Lemma 11, we have $S_k(G) \leq k(r-1) + \frac{n}{2}(1+\sqrt{k})$. So it is sufficient to show that

$$g(r) := 2k(r-1) + n(1+\sqrt{k}) - rn - k(k+1) \leq 0.$$

As $n/2 \leq k$, g is increasing with respect to r. Thus

$$g(r) \leq g(3n/4) = -3n^2/4 + n(3k/2 + \sqrt{k} + 1) - k(k+3).$$

Now, $g(3n/4)$ as a quadratic form in n has a negative discriminant, and thus it is negative. Finally assume that $r > 3n/4$. In view of Lemma 9 (ii) it suffices to show that

$$2n^2 \leq (3n-4k)r + 2kn + k^2 + k. \tag{5}$$

Since $k < 3n/4$, the right hand side of (5) is increasing in r, so it is enough to show that (5) holds for $r = 3n/4$ but this amounts to show that $n^2/4 - kn + k^2 + k \geq 0$ which always holds. This completes the proof. □

4 Proof of Conjecture 1 for $k = 2$

In this section, we prove that Conjecture 1 is true for $k = 2$.

Lemma 13. *Let G be a graph and $v \in V(G)$ with $q_2(G) \geq d(v)$. If the graph G' is obtained from G by duplicating v, i.e. adding a new vertex v' with $N(v) = N(v')$, then $S_2(G') - e(G') \leq S_2(G) - e(G)$.*

Proof. Let Q and Q' be the signless Laplacian matrices of G and G', respectively. Let d be the common value of $d(v)$ and $d(v')$. Then the corresponding rows of v and v' in $Q' - dI$ are the same. Thus the nullity of $Q' - dI$ is one more than the nullity of $Q - dI$. So the multiplicity of d as an eigenvalue of Q' is one more than that of Q. On the other hand, from Theorem 2 it follows that $q_2(G') \geq q_2(G) \geq d$. Since $S_n(G') = S_n(G) + 2d$, it turns out that adding v' increases the sum of the two largest eigenvalue by at most d, that is $S_2(G') \leq S_2(G) + d$. The result now follows. □

Since $\mu_1(G) + \mu_2(G) \leq e(G) + 3$ by [10], using the fact that signless Laplacian matrix and Laplacian matrix are similar for a bipartite graph we have the following.

Lemma 14. *If G is a bipartite graph, then $S_2(G) \leq e(G) + 3$.*

Lemma 15. *If Conjecture 1 is false for $k = 2$, then there exists a counterexample G for which $S_2(H) > e(H)$ for every subgraph H of G. In particular, G contains neither $H = 4K_2$ nor $H = 3S_3$ as a subgraph.*

Proof. Let G be a counterexample for Conjecture 1 with $k = 2$ having a minimum number of edges. If G has a nonempty subgraph H with $S_2(H) \leq e(H)$, then by Theorem 3, $e(G) + 3 < S_2(G) \leq S_2(H) + S_2(G - E(H))$. This implies that $S_2(G - E(H)) > e(G - E(H)) + 3$, which contradicts the minimality of $e(G)$. Noting that for $H = 4K_2$ or $H = 3S_3$, one has $S_2(H) = e(H)$, completes the proof. □

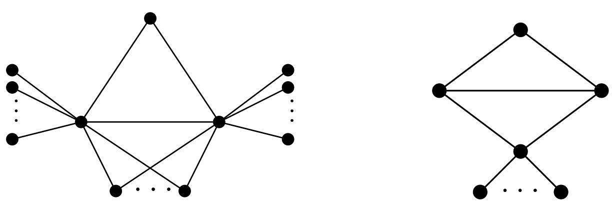
Now from Lemma 15 we see that in order to prove the main result of this section, it is sufficient to consider only graphs G whose matching number $m(G)$ is at most 3.

Lemma 16. *Let G be a graph with $m(G) = 1$. Then $S_2(G) \leq e(G) + 3$.*

Proof. Let $n = |V(G)|$. Since $m(G) = 1$, it is easily checked that either $G = S_a \cup (n - a)K_1$ for some a, $1 \leq a \leq n$ or $G = K_3 \cup (n - 3)K_1$. By Lemma 7, the assertion holds. □

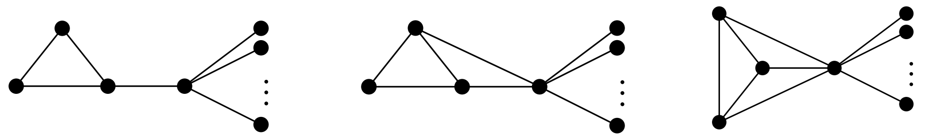
Lemma 17. *Let G be a graph with $m(G) = 2$. Then $S_2(G) \leq e(G) + 3$.*

Proof. We may assume that G is a connected graph by Lemma 4. First suppose that G has a subgraph $H = K_3$ with $V(H) = \{u, v, w\}$. If every edge of G has at least one endpoint in $V(H)$, then G is a graph of the following form:



By Lemma 13, we may assume that, in the right graph, the number of degree 1 vertices and in the left graph the number of degree 1 vertices in either side and the number of degree 2 vertices at the bottom are at most one. Such a graph has at most 6 vertices and the result follows from Lemma 6.

Hence assume that there exists an edge $e = \{a, b\}$ whose endpoints are in $V(G) - V(H)$. Let $M = V(G) - \{a, b, u, v, w\}$. Since $m(G) = 2$, there are no edges between $V(H)$ and M. Therefore, G has one of the following form:

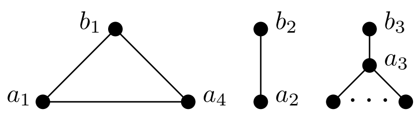


Again by Lemma 13, we only need to prove the assertion when the number of degree 1 vertices is at most 1 in which case the result follows by Lemma 6.

Next assume that G has no K_3 as a subgraph. Suppose that $e_1 = \{a_1, b_1\}$ and $e_2 = \{a_2, b_2\}$ are two independent edges in G. Since G contains neither $3K_2$ nor K_3 as subgraphs, $M = V(G) - \{a_1, b_1, a_2, b_2\}$ is an independent set and at least one of the two endpoints of e_i has no neighbors in M for $i = 1, 2$. Assume those endpoints to be b_1 and b_2. If b_1 and b_2 are adjacent, then $|M| \geq 2$ yields that all vertices in M are adjacent to only one of the two vertices a_1 and a_2, say a_1. This implies that G is a bipartite graph with the vertex set partition $\{\{a_1, b_2\}, V(G) - \{a_1, b_2\}\}$. Now assume that b_1 and b_2 are not adjacent. If a_1 and a_2 are adjacent, then G is a tree. Otherwise, G is a bipartite graph and the proof is complete by Lemma 14. □

Lemma 18. *Let G be a graph with $m(G) = 3$. Then $S_2(G) \leq e(G) + 3$.*

Proof. We first assume that G is a connected graph that has $K_3 + 2K_2$ as a subgraph. So G contains the following graph as a subgraph with possibly some edges between the vertices $\{a_1, a_2, a_3, a_4, b_1, b_2, b_3\}$ which contain neither $3S_3$ nor $4K_2$.



Again it suffices to prove the assertion when the number of degree 1 vertices is at most 1 for which the result follows from Lemma 6.

Then suppose that G has no subgraph $K_3 + 2K_2$. Let $e_1 = \{a_1, b_1\}$, $e_2 = \{a_2, b_2\}$ and $e_3 = \{a_3, b_3\}$ be three independent edges in G. Since $m(G) = 3$, $M = V(G) - V(\{e_1, e_2, e_3\})$ is an independent set. Since G has neither $4K_2$ nor $K_3 + 2K_2$ as subgraphs, either $N(a_i) \cap M = \emptyset$ or $N(b_i) \cap M = \emptyset$, for $i = 1, 2, 3$. With no loss of generality, we may assume that $N(M) \subseteq \{a_1, a_2, a_3\}$. If $|N(M)| \leq 2$, then applying Lemma 13, we may assume that G has at most 10 vertices and so the result follows Lemma 6. Hence, assume that $|N(M)| = 3$. We have $N(M) = \{a_1, a_2, a_3\}$. Since G has no $3S_3$, the bipartite subgraph $G - \{b_1, b_2, b_3\}$ has no any matching of size 3. By Hall's theorem, there exists a subset of $\{a_1, a_2, a_3\}$ with 2 elements, say $\{a_2, a_3\}$, such that $|N(\{a_2, a_3\}) \cap M| = 1$. That means that all other vertices of M are adjacent to a_1 only and again we are done by Lemmas 6 and 13. □

Now from Lemmas 15, 16, 17 and 18, the main result of this section follows:

Theorem 19. *Let G be a graph with at least two vertices. Then $S_2(G) \leq e(G) + 3$.*

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