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Upper bounds for the sum of Laplacian eigenvalues of graphs

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ABSTRACT

Let G be a graph with n vertices and $e(G)$ edges, and let $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G) = 0$ be the Laplacian eigenvalues of G. Let $S_k(G) = \sum_{i=1}^{k} \mu_i(G)$, where $1 \leq k \leq n$. Brouwer conjectured that $S_k(G) \leq e(G) + \binom{k+1}{2}$ for $1 \leq k \leq n$. It has been shown in Haemers et al. [7] that the conjecture is true for trees. We give upper bounds for $S_k(G)$, and in particular, we show that the conjecture is true for unicyclic and bicyclic graphs.

1. Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The Laplacian matrix of G is defined as $\mathbf{L}(G) = \mathbf{D}(G) - \mathbf{A}(G)$, where $\mathbf{D}(G)$ is the diagonal matrix of vertex degrees of the graph G, and $\mathbf{A}(G)$ is the adjacency matrix of G. Let $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G) = 0$ be the Laplacian eigenvalues of G, i.e., the eigenvalues of $\mathbf{L}(G)$, where $n = |V(G)|$. Let $S_k(G) = \sum_{i=1}^{k} \mu_i(G)$, where $1 \leq k \leq n$.

Let d_v be the degree of v in G. Let $d_i^*(G) = |\{v \in V(G) : d_v \geq i\}|$ for $i = 1, 2, \ldots, n$. Obviously $d_1^*(G) \geq d_2^*(G) \geq \cdots \geq d_n^*(G)$. If G is a graph with n vertices, then the Grone–Merris conjecture states that [6]

$$S_k(G) \leq \sum_{i=1}^{k} d_i^*(G)$$

for $1 \leq k \leq n$. Very recently, it was proven by Bai [1].

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Let $e(G) = |E(G)|$ for the graph G. As a variation of the Grone–Merris conjecture, Brouwer proposed the following conjecture, see [3,7].

Conjecture 1.1. *Let G be a graph with n vertices. Then*

$$S_k(G) \leq e(G) + \binom{k+1}{2}$$

for $1 \leq k \leq n$.

Brouwer verified Conjecture 1.1 by computer for all graphs with at most 10 vertices, see [7]. For $k = n - 1$ or n, Conjecture 1.1 follows trivially because $S_k(G) = 2e(G)$. For $k = 1$, Conjecture 1.1 follows from the well-known inequality $\mu_1(G) \leq n$, see [5]. Haemers et al. [7] showed that Conjecture 1.1 is true for all graphs when $k = 2$ and is true for trees. See [3] for progress of Conjecture 1.1.

Recall that an n-vertex connected graph G is unicyclic (bicyclic, respectively) if $e(G) = n$ ($e(G) = n + 1$, respectively).

In this paper, we give various upper bounds for $S_k(G)$, and in particular, we show that Conjecture 1.1 is true for unicyclic and bicyclic graphs.

2. Preliminaries

Let $\lambda_1(\mathbf{A}) \geq \lambda_2(\mathbf{A}) \geq \cdots \geq \lambda_n(\mathbf{A})$ be the eigenvalues of the $n \times n$ symmetric matrix $\mathbf{A}$.

Lemma 2.1 [4]**.** *Let $\mathbf{A}$ and $\mathbf{B}$ be two real $n \times n$ symmetric matrices. Then*

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

for $1 \leq k \leq n$.

For a graph G with $E' \subseteq E(G)$, let $G - E'$ be the graph obtained from G by deleting the edges in E'. If $E' = \{e\}$, then we write $G - e$ for $G - \{e\}$.

Let $G \cup H$ be the vertex-disjoint union of the graphs G and H. For integer $k \geq 1$, let kG be the vertex-disjoint union of k copies of the graph G.

Let K_n be the complete graph with n vertices. Let $K_{1,s}$ be the star on $s + 1$ vertices, in particular, $K_{1,0} = K_1$.

Lemma 2.2. *Let H be a subgraph of graph G, and $|V(H)| = n_1 \geq 2$. Then*

$$S_k(G) \leq S_k(H) + 2(e(G) - e(H))$$

for $1 \leq k \leq n_1$.

Proof. If $G = H$, then the result is obvious. Suppose in the following that H is a proper subgraph of G. Let $1 \leq k \leq n_1$ and $E(G) \backslash E(H) = \{e_1, e_2, \ldots, e_r\}$, where $r = e(G) - e(H)$. Let $|V(G)| = n$. By Lemma 2.1,

$$\begin{aligned}
S_k(G) &\leq S_k(G - e_1) + S_k(K_2 \cup (n-2)K_1) \\
&= S_k(G - e_1) + 2 \\
&\leq S_k(G - e_1 - e_2) + 2 + 2 \\
&\leq \cdots \\
&\leq S_k(G - e_1 - e_2 - \cdots - e_r) + 2r \\
&= S_k(H \cup (n - n_1)K_1) + 2(e(G) - e(H)) \\
&= S_k(H) + 2(e(G) - e(H)),
\end{aligned}$$

as desired. □

Obviously, the upper bound for $S_k(G)$ given in Lemma 2.2 is better than the trivial upper bound $2e(G)$ if and only if $S_k(H) < 2e(H)$ (which implies that $k \leq n_1 - 2$).

Lemma 2.3 [7]. *Let G be a tree with n vertices. Then* $S_k(G) \leq e(G) + 2k - 1$ *for* $1 \leq k \leq n$.

Lemma 2.4 [7]. *Let G be a graph with* $n \geq 2$ *vertices. Then* $S_2(G) \leq e(G) + 3$.

3. Upper bounds for $S_k(G)$

In this section, we give various upper bounds for $S_k(G)$.

Recall that the clique number of a graph G is the number of vertices of a maximum complete subgraph of G.

Proposition 3.1. *Let G be a graph with clique number* $\omega \geq 3$. *Then*

$$S_k(G) \leq 2e(G) + \omega(k - \omega + 1)$$

for $1 \leq k \leq \omega - 2$.

Proof. Obviously, K_ω is a subgraph of G. Note that the Laplacian eigenvalues of K_ω are ω with multiplicity $\omega - 1$, and 0. If $1 \leq k \leq \omega - 2$, then $S_k(G) = k\omega$, and thus by Lemma 2.2,

$$\begin{aligned} S_k(G) &\leq S_k(K_\omega) + 2\left(e(G) - \binom{\omega}{2}\right) \\ &= k\omega + 2\left(e(G) - \binom{\omega}{2}\right) \\ &= 2e(G) + \omega(k - \omega + 1), \end{aligned}$$

as desired. □

Proposition 3.2. *Let G be a graph with maximum degree* $\Delta \geq 2$. *Then*

$$S_k(G) \leq 2e(G) - \Delta + k$$

for $1 \leq k \leq \Delta - 1$.

Proof. Obviously, $K_{1,\Delta}$ is a subgraph of G. Note that the Laplacian eigenvalues of $K_{1,\Delta}$ are $\Delta + 1$, 1 with multiplicity $\Delta - 1$, and 0. If $1 \leq k \leq \Delta - 1$, then $S_k(G) = \Delta + k$, and thus by Lemma 2.2,

$$\begin{aligned} S_k(G) &\leq S_k(K_{1,\Delta}) + 2(e(G) - \Delta) \\ &= (\Delta + k) + 2(e(G) - \Delta) \\ &= 2e(G) - \Delta + k, \end{aligned}$$

as desired. □

A matching M of the graph G is a subset of $E(G)$ such that no two edges in M share a common vertex. The matching number of G is the maximum number of edges of a matching in G.

Proposition 3.3. *Let G be a graph with matching number* $m \geq 2$. *Then*

$$S_k(G) \leq 2e(G) - 2m + 2k$$

for $1 \leq k \leq m - 1$.

Proof. Obviously, mK_2 is a subgraph of G. Note that the Laplacian eigenvalues of mK_2 are 2 with multiplicity m, and 0 with multiplicity m. If $1 \le k \le m-1$, then $S_k(G) = 2k$, and thus by Lemma 2.2,

$$\begin{aligned} S_k(G) &\le S_k(mK_2) + 2(e(G) - m) \\ &= 2k + 2(e(G) - m) \\ &= 2e(G) - 2m + 2k, \end{aligned}$$

as desired. □

Proposition 3.4. *Let G be a graph with n vertices and without isolated vertices. Then*

$$S_k(G) \le 2e(G) - n + 2k$$

for $1 \le k \le n$.

Proof. Suppose first that G is connected. Let T be a spanning tree of G. By Lemmas 2.2 and 2.3,

$$\begin{aligned} S_k(G) &\le S_k(T) + 2(e(G) - e(T)) \\ &\le (e(T) + 2k - 1) + 2(e(G) - n + 1) \\ &= 2e(G) - n + 2k. \end{aligned}$$

Now suppose that G is not connected. Let $G_1, G_2, \ldots, G_t$ be all the components of G. Suppose that k_i of the first k largest Laplacian eigenvalues of G are Laplacian eigenvalues of G_i, where $0 \le k_i \le k$, $1 \le i \le t$, and $\sum_{i=1}^{t} k_i = k$. Suppose without loss of generality that $k_1, k_2, \ldots, k_r > 0 = k_{r+1} = \cdots = k_t$, where $1 \le r \le t$. Then $S_k(G) = \sum_{i=1}^{r} S_{k_i}(G_i)$. Let $H = \cup_{i=1}^{r} G_i$. Obviously, $S_k(G) = S_k(H)$. Let $n_i = |V(G_i)|$ for $i = 1, 2, \ldots, t$. By the proof above, we have $S_{k_i}(G_i) \le 2e(G_i) - n_i + 2k_i$ for $1 \le i \le r$. Then

$$\begin{aligned} S_k(G) &= S_k(H) = \sum_{i=1}^{r} S_{k_i}(G_i) \\ &\le \sum_{i=1}^{r} 2e(G_i) - \sum_{i=1}^{r} n_i + \sum_{i=1}^{r} 2k_i \\ &= 2e(H) - |V(H)| + 2k. \end{aligned}$$

Note that $e(G_i) \ge 1$ for $r+1 \le i \le t$ since G contains no isolated vertices. For $r+1 \le i \le t$, $e(G_i) - n_i \ge -1$, and thus $2e(G_i) - n_i \ge 0$, implying that $2e(G) - n \ge 2e(H) - |V(H)|$. Then the result follows. □

The upper bound for $S_k(G)$ given in Proposition 3.4 is better than the trivial upper bound $2e(G)$ if and only if $1 \le k \le \lfloor \frac{n-1}{2} \rfloor$.

If $G = \frac{n}{2}K_2$ for even n, then equality in Proposition 3.4 holds for $1 \le k \le \frac{n}{2}$.

For a connected graph on n vertices with $1 \le k \le n-2$, it was shown in [9] that

$$S_k(G) \le \frac{2e(G)k + \sqrt{e(G)k(n-k-1)(n^2 - n - 2e(G))}}{n-1}$$

with equality if and only if $G \cong K_{1,n-1}$ or K_n when $k = 1$, and $G \cong K_n$ when $2 \le k \le n-2$.

If $G = K_{1,n-1}$, then the bound in Proposition 3.4 is better than the one mentioned above in [9] for $2 \le k \le n-3$, and if $G = K_n$, then the bound mentioned above in [9] is better than the one in Proposition 3.4 for $1 \le k \le n-2$. Thus these two bounds are incomparable in general.

For a graph G with n vertices, let $\overline{G}$ be the complement of G. Note that $\mathbf{L}(G)+\mathbf{L}(\overline{G})=\mathbf{L}(K_n)$. By Lemma 2.1,

$$S_k(G)+S_k(\overline{G})\geq kn$$

for $1\leq k\leq n-1$, and

$$S_k(G)+S_k(\overline{G})\geq n(n-1)$$

for $k=n$. If both G and $\overline{G}$ have no isolated vertices, then since $e(G)+e(\overline{G})=\frac{n(n-1)}{2}$, we have by Proposition 3.4 that

$$S_k(G)+S_k(\overline{G})\leq n^2-3n+4k$$

for $1\leq k\leq n$.

Proposition 3.5. *Let G be a graph with n vertices, of which n_1 are not isolated vertices. Then*

$$S_k(G)\leq e(G)+\binom{k+1}{2}$$

for $1\leq k\leq n$ if $9-8(n_1-e(G))<0$, and for $\left\lceil\frac{3+\sqrt{9-8(n_1-e(G))}}{2}\right\rceil\leq k\leq n$ if $9-8(n_1-e(G))\geq 0$.

Proof. If $n_1=0$, then G is an empty graph, and thus the result is obvious. Obviously, $n_1\neq 1$. Suppose that $n_1\geq 2$. Let H be the graph obtained from G by deleting all isolated vertices. Obviously, $S_k(G)=S_k(H)$ for $1\leq k\leq n_1$, and $S_k(G)=S_{n_1}(H)$ for $n_1+1\leq k\leq n$.

For $1\leq k\leq n_1$ if $9-8(n_1-e(H))<0$, and for $\left\lceil\frac{3+\sqrt{9-8(n_1-e(H))}}{2}\right\rceil\leq k\leq n_1$ if $9-8(n_1-e(H))\geq 0$, we have

$$2e(H)-n_1+2k\leq e(H)+\binom{k+1}{2},$$

and thus by Proposition 3.4,

$$S_k(G)=S_k(H)\leq 2e(H)-n_1+2k\leq e(H)+\binom{k+1}{2}=e(G)+\binom{k+1}{2}.$$

For $n_1+1\leq k\leq n$, since $S_{n_1}(H)=2e(H)<e(H)+\binom{n_1+1}{2}$, we have

$$S_k(G)=S_{n_1}(H)<e(H)+\binom{n_1+1}{2}<e(G)+\binom{k+1}{2}.$$

The result follows. □

4. Conjecture 1.1 for unicyclic and bicyclic graphs

If G is an n-vertex unicyclic graph, then $e(G)=n$, and thus $\left\lceil\frac{3+\sqrt{9-8(n-e(G))}}{2}\right\rceil=3$. By Proposition 3.5, we have Conjecture 1.1 is true for n-vertex unicyclic graphs when $3\leq k\leq n$. Recall that Conjecture 1.1 is true for $k=2$, see [7]. Thus we have

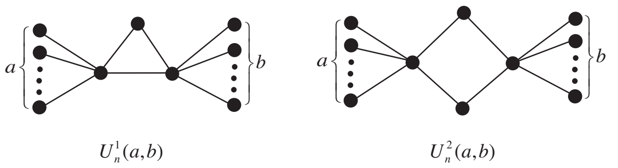

Fig. 1. The graphs $U_n^1(a, b)$ and $U_n^2(a, b)$.

Corollary 4.1. *Conjecture 1.1 is true for unicyclic graphs.*

In the rest of this paper, we show that Conjecture 1.1 is true for bicyclic graphs. If G is an n-vertex bicyclic graph, then $e(G) = n + 1$, and thus $\left\lceil \frac{3+\sqrt{9-8(n-e(G))}}{2} \right\rceil = 4$. By Proposition 3.5, we have Conjecture 1.1 is true for n-vertex bicyclic graphs when $4 \le k \le n$. By the fact that Conjecture 1.1 is true for $k = 2$ (see [7]), to show Conjecture 1.1 is true for n-vertex bicyclic graphs, we need only to show that it is true for bicyclic graphs when $k = 3$.

We need some lemmas.

Lemma 4.1 [2]. *Let G be a graph on n vertices with degree sequence $\delta_1 \ge \delta_2 \ge \cdots \ge \delta_n$. If $G \ncong K_s \cup (n-s)K_1$, then $\mu_s(G) \ge \delta_s - s + 2$ for $1 \le s \le n$.*

Let $\phi(G, x)$ be the characteristic polynomial of $\mathbf{L}(G)$.

A pendent vertex is a vertex of degree one. A pendent edge is an edge incident to a pendent vertex.

Let $U_n^1(a, b)$ be the graph obtained by attaching a and b pendent vertices to two vertices of a triangle, respectively, where $a+b = n-3$, $n \ge 4$, $a \ge b \ge 0$. Let $U_n^2(a, b)$ be the graph obtained by attaching a and b pendent vertices to two non-adjacent vertices of a quadrangle, respectively, where $a+b = n-4$, $n \ge 5$, $a \ge b \ge 0$. The graphs $U_n^1(a, b)$ and $U_n^2(a, b)$ are presented in Fig. 1.

Lemma 4.2. *For $n \ge 9$, $a \ge b \ge 0$, $\mu_3(U_n^1(a, b)) < 2$ and $\mu_3(U_n^2(a, b)) = 2$.*

Proof. By direct calculation, we have

$$\phi(U_n^1(a, b), x) = x(x-1)^{n-5}f(x),$$

$$\phi(U_n^2(a, b), x) = x(x-2)(x-1)^{n-6}g(x),$$

where

$$f(x) = x^4 - (n+5)x^3 + (5n+ab+7)x^2 - (7n+2ab+3)x + 3n,$$

$$g(x) = x^4 - (n+4)x^3 + (5n+ab+1)x^2 - (6n+2ab-2)x + 2n.$$

Let $x_1 \ge x_2 \ge x_3 \ge x_4$ be the roots of $f(x) = 0$, and $y_1 \ge y_2 \ge y_3 \ge y_4$ be the roots of $g(x) = 0$.

By Lemma 4.1, we have $\mu_2(U_n^1(a, b)) \ge 2 > 1$, and thus $\mu_2(U_n^1(a, b)) = x_2$, and $\mu_3(U_n^1(a, b)) = x_3$ or 1. Note that $f(2) = n-2 > 0$ and $f(1) = -ab \le 0$. Then $x_3 < 2$, and thus $\mu_3(U_n^1(a, b)) < 2$.

By Lemma 4.1, we have $\mu_1(U_n^2(a, b)) \ge 3$, and thus $\mu_1(U_n^2(a, b)) = y_1$, $\mu_2(U_n^2(a, b)) = y_2$ or 2. Note that $g(2) = 2n-8 > 0$ and $g(1) = -ab \le 0$. Then $y_3 < 2 < y_2$, and thus $\mu_2(U_n^2(a, b)) = y_2$ and $\mu_3(U_n^2(a, b)) = 2$. $\square$

Lemma 4.3. *Let G be a graph with $n \ge 11$ vertices. Suppose that there are two edges $e_1, e_2 \in E(G)$ such that $G - \{e_1, e_2\} = H \cup K_2$, where $H = U_n^i(a, b)$ for some integers a, b with $a+b = n-2-i$, $a \ge b \ge 0$ and $i = 1, 2$. Then $S_3(G) \le e(G) + 6$.*

Proof. By Lemma 4.2, the first three largest Laplacian eigenvalues of $H \cup K_2$ are $\mu_1(H)$, $\mu_2(H)$ and 2, i.e., $S_3(H \cup K_2) = S_2(H) + 2$. By Lemmas 2.2 and 2.4,

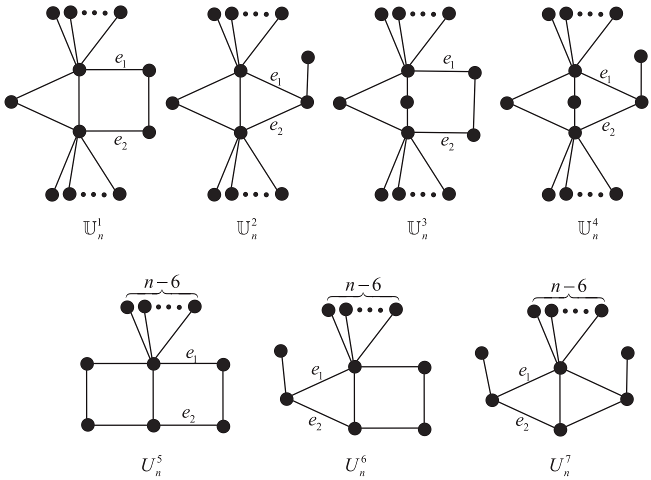

Fig. 2. The structures of graphs in $\mathbb{U}_n^1$, $\mathbb{U}_n^2$, $\mathbb{U}_n^3$, and $\mathbb{U}_n^4$, and graphs U_n^5, U_n^6, and U_n^7.

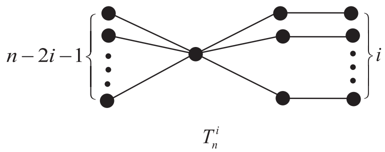

Fig. 3. The tree T_n^i with $i = 0, 1, 2, 3$.

$$
\begin{aligned}
S_3(G) &\le S_3(H \cup K_2) + 2 \cdot 2 \\
&= S_2(H) + 6 \\
&\le (e(H) + 3) + 6 \\
&= e(G) + 6,
\end{aligned}
$$

as desired. □

For $n \ge 11$, we define four classes of n-vertex bicyclic graphs, denoted by $\mathbb{U}_n^1$, $\mathbb{U}_n^2$, $\mathbb{U}_n^3$, and $\mathbb{U}_n^4$, for which the structures of graphs in them are given in Fig. 2. We also need three n-vertex bicyclic graphs, denoted by U_n^5, U_n^6, and U_n^7 for $n \ge 11$, see also Fig. 2.

Lemma 4.4. *Let $G \in \cup_{i=1}^4 \mathbb{U}_n^i$, or $G = U_n^i$ with $i = 5, 6, 7$, where $n \ge 11$. Then $S_3(G) \le e(G) + 6$.*

Proof. For each graph G, let e_1, e_2 be the edges as labeled in Fig. 2. Then the result follows from Lemma 4.3. □

Lemma 4.5 [8]. *Let G be a graph. Then $\mu_1(G) \le \max\{d_u + m_u : u \in V(G)\}$, where $m_u = \frac{1}{d_u} \sum_{uv \in E(G)} d_v$.*

For $i = 0, 1, 2, 3$, let T_n^i be the tree obtained by attaching i paths with two vertices to the central vertex of $K_{1,n-2i-1}$, where $n \ge 2i + 1$, see Fig. 3. In particular, $T_n^0 = K_{1,n-1}$.

Lemma 4.6. *(i) For $n \ge 6$, we have $1 < \mu_2(T_n^2) < 2.7$, $S_2(T_n^2) < e(T_n^2) + 2$. (ii) For $n \ge 7$, we have $1 < \mu_2(T_n^3) < 2.7$, $S_2(T_n^3) < e(T_n^3) + 2$.*

Proof. By Lemma 4.1, $\mu_2(T_n^2), \mu_2(T_n^3) \geq 2 > 1$.

By direct calculation, we have

$$\phi(T_n^2, x) = x(x-1)^{n-6}f(x),$$

$$\phi(T_n^3, x) = x(x-1)^{n-8}g(x),$$

where

$$f(x) = x^5 - (n+4)x^4 + (6n-1)x^3 - (11n-14)x^2 + (6n-5)x - n,$$

$$g(x) = x^7 - (n+6)x^6 + (9n+3)x^5 - (30n-42)x^4 + (45n-87)x^3$$
$$-(30n-48)x^2 + (9n-8)x - n.$$

Let $x_1 \geq x_2 \geq x_3 \geq x_4 \geq x_5$ be the roots of $f(x) = 0$, and $y_1 \geq y_2 \geq y_3 \geq y_4 \geq y_5 \geq y_6 \geq y_7$ be the roots of $g(x) = 0$. Obviously, $\sum_{i=1}^{5} x_i = n + 4$ and $\sum_{i=1}^{7} y_i = n + 6$.

By Lemma 4.1, $\mu_1(T_n^2) \geq n-2$, $\mu_2(T_n^2) \geq 2$, and $\mu_1(T_n^3) \geq n-3$, $\mu_2(T_n^3) \geq 2$. Thus $\mu_1(T_n^2) = x_1$, $\mu_2(T_n^2) = x_2$, and $\mu_1(T_n^3) = y_1$, $\mu_2(T_n^3) = y_2$. It is easily checked that both $f(x)$ and $g(x)$ are increasing for $x \leq 0.38$, and thus $f(x) \leq f(0.38) < 0$ and $g(x) \leq g(0.38) < 0$, implying that $x_5 > 0.38$ and $y_7 > 0.38$.

(i) Note that $f(2.7) < 0$. Thus $x_2 < 2.7 < x_1$, $x_4 < 2.7 < x_3$, or $x_5 > 2.7$. If $x_5 > 2.7$, then

$$n + 4 = x_1 + x_2 + x_3 + x_4 + x_5$$
$$> (n-2) + 2.7 + 2.7 + 2.7 + 2.7 = n + 8.8,$$

a contradiction. If $x_4 < 2.7 < x_3$, then

$$n + 4 = x_1 + x_2 + x_3 + x_4 + x_5$$
$$> (n-2) + 2.7 + 2.7 + 0.38 + 0.38 = n + 4.16,$$

a contradiction. Thus $\mu_2(T_n^2) = x_2 < 2.7$.

By direct calculation, $S_2(T_n^2) < e(T_n^2) + 2$ for $6 \leq n \leq 9$. If $n \geq 10$, then by Lemma 4.5, $\mu_1(T_n^2) \leq n - 2 + \frac{2}{n-3}$, and thus

$$\begin{aligned} S_2(T_n^2) &= \mu_1(T_n^2) + \mu_2(T_n^2) \\ &< \left(n - 2 + \frac{2}{n-3}\right) + 2.7 \\ &= n + 0.7 + \frac{2}{n-3} \\ &\leq n + 0.7 + \frac{2}{10-3} \\ &< n + 1 = e(T_n^2) + 2. \end{aligned}$$

(ii) Note that $g(2.7) < 0$. Thus $y_2 < 2.7 < y_1$, $y_4 < 2.7 < y_3$, $y_6 < 2.7 < y_5$, or $y_7 > 2.7$. If $y_7 > 2.7$, then

$$n + 6 = y_1 + y_2 + y_3 + y_4 + y_5 + y_6 + y_7$$
$$> (n-3) + 2.7 + 2.7 + 2.7 + 2.7 + 2.7 + 2.7 = n + 13.2,$$

a contradiction. If $y_6 < 2.7 < y_5$, then

$$\begin{aligned} n+6 &= y_1+y_2+y_3+y_4+y_5+y_6+y_7 \\ &> (n-3)+2.7+2.7+2.7+2.7+0.38+0.38 = n+8.56, \end{aligned}$$

a contradiction. If $y_4 < 2.7 < y_3$ for $n \geq 18$, then since $g(2.5) > 0$, we have $y_4 > 2.5$, and thus

$$\begin{aligned} n+6 &= y_1+y_2+y_3+y_4+y_5+y_6+y_7 \\ &> (n-3)+2.7+2.7+2.5+0.38+0.38+0.38 = n+6.04, \end{aligned}$$

a contradiction. By direct calculation, $y_2 < 2.7 < y_1$ for $7 \leq n \leq 17$. Thus $\mu_2(T_n^3) = y_2 < 2.7$.

By Lemma 4.5, $\mu_1(T_n^3) \leq n-3+\frac{3}{n-4}$, and thus

$$\begin{aligned} S_2(T_n^3) &= \mu_1(T_n^3)+\mu_2(T_n^3) \\ &< \left(n-3+\frac{3}{n-4}\right)+2.7 \\ &= n-0.3+\frac{3}{n-4} \\ &\leq n-0.3+\frac{3}{7-4} \\ &< n+1 = e(T_n^3)+2. \end{aligned}$$

The result follows. □

Lemma 4.7. *Let G be a bicyclic graph with $e_1, e_2, e_3 \in E(G)$. Suppose that each bicyclic graph H with $|V(H)| < |V(G)|$ satisfies $S_3(H) \leq e(H)+6$.*

(i) If $G-e_1$ consists of two nontrivial components, then $S_3(G) \leq e(G)+6$.
(ii) If $G-\{e_2, e_3\}$ consists of two components with at least three vertices, then $S_3(G) \leq e(G)+6$.

Proof. (i) Let G_1 and G_2 be the two components of $G-e_1$. Then $G-e_1=G_1 \cup G_2$. It is easily seen that either one of them is a tree and the other one is a bicyclic graph, or both of them are unicyclic graphs. Note that Conjecture 1.1 is true for trees (see [7]) and unicyclic graphs (see Corollary 4.1), and $|V(G_i)|<|V(G)|$ for $i=1, 2$. We have $S_3(G_i) \leq e(G_i)+6$ for $i=1, 2$. If $S_3(G_1 \cup G_2) = S_3(G_1)$, then by Lemma 2.2,

$$\begin{aligned} S_3(G) &\leq S_3(G_1 \cup G_2)+2 \\ &= S_3(G_1)+2 \\ &\leq (e(G_1)+6)+2 \\ &= e(G_1)+8 \leq e(G)+6. \end{aligned}$$

If $S_3(G_1 \cup G_2) = S_3(G_2)$, then as above, we have $S_3(G) \leq e(G)+6$. Suppose that $S_3(G_1 \cup G_2) \neq S_3(G_1), S_3(G_2)$. Suppose without loss of generality that the first three largest Laplacian eigenvalues of $G_1 \cup G_2$ are $\mu_1(G_1)$, $\mu_2(G_1)$, and $\mu_1(G_2)$, i.e., $S_3(G_1 \cup G_2) = S_2(G_1)+S_1(G_2)$. By Lemmas 2.2 and 2.4,

$$\begin{aligned} S_3(G) &\leq S_3(G_1 \cup G_2)+2 \\ &= S_2(G_1)+S_1(G_2)+2 \\ &\leq (e(G_1)+3)+|V(G_2)|+2 \\ &\leq (e(G_1)+3)+(e(G_2)+1)+2 \\ &= e(G)+5. \end{aligned}$$

Thus (i) follows.

(ii) Let G_3 and G_4 be the two components of $G - \{e_2, e_3\}$. Then $G - \{e_2, e_3\} = G_3 \cup G_4$. It is easily seen that one of them is a tree and the other one is a unicyclic graph. Since Conjecture 1.1 is true for trees and unicyclic graphs, we have $S_3(G_i) \le e(G_i) + 6$ for $i = 3, 4$. If $S_3(G_3 \cup G_4) = S_3(G_3)$, then by Lemma 2.2,

$$\begin{aligned} S_3(G) &\le S_3(G_3 \cup G_4) + 2 \cdot 2 \\ &= S_3(G_3) + 4 \\ &\le (e(G_3) + 6) + 4 \\ &= e(G_3) + 10 \le e(G) + 6. \end{aligned}$$

If $S_3(G_3 \cup G_4) = S_3(G_4)$, then as above, we have $S_3(G) \le e(G) + 6$. Suppose that $S_3(G_3 \cup G_4) \ne S_3(G_3), S_3(G_4)$. Suppose without loss of generality that the first three largest Laplacian eigenvalues of $G_3 \cup G_4$ are $\mu_1(G_3)$, $\mu_2(G_3)$, and $\mu_1(G_4)$, i.e., $S_3(G_3 \cup G_4) = S_2(G_3) + S_1(G_4)$. By Lemmas 2.2 and 2.4,

$$\begin{aligned} S_3(G) &\le S_3(G_3 \cup G_4) + 2 \cdot 2 \\ &= S_2(G_3) + S_1(G_4) + 4 \\ &\le (e(G_3) + 3) + |V(G_4)| + 4 \\ &\le (e(G_3) + 3) + (e(G_4) + 1) + 4 \\ &= e(G) + 6. \end{aligned}$$

Then (ii) follows. □

Lemma 4.8. *Let G be a bicyclic graph. Then $S_3(G) \le e(G) + 6$.*

Proof. Let $n = |V(G)|$. Recall that Conjecture 1.1 is true for all graphs with at most ten vertices (see [7]). Thus the result holds for $n \le 10$. Suppose that the result is not true. Let G be a counterexample with the minimum number of vertices, i.e., $S_3(G) > e(G) + 6$ with $n \ge 11$.

Case 1. There are two vertex-disjoint cycles in G. Note that each edge, say e_1, lying on the unique path joining the two cycles is a cut edge. Obviously, the two components of $G - e_1$ are both unicyclic graphs (which are nontrivial). By Lemma 4.7 (i), we have $S_3(G) \le e(G) + 6$, a contradiction.

Case 2. There are two cycles in G with a common vertex. Let $C^{(1)}$ and $C^{(2)}$ be the two cycles of G with a unique common vertex u.

If there is a non-pendent edge, say e_2, outside the cycles in G, then $G - e_2$ consists of two nontrivial components, and thus by Lemma 4.7 (i), we have $S_3(G) \le e(G) + 6$, a contradiction. Thus every edge outside the cycles of G is a pendent edge.

Denote by u_1 and u_2 the two neighbors of u in $C^{(1)}$. Then $G - \{uu_1, uu_2\}$ consists of two components, one of which containing u_1, denoted by G_1, is a tree, and the other one containing u is a unicyclic graph. If $e(G_1) \ge 2$, then there are at least three vertices in each component of $G - \{uu_1, uu_2\}$, and thus by Lemma 4.7 (ii), we have $S_3(G) \le e(G) + 6$, a contradiction. Thus $e(G_1) < 2$. Note that $e(G_1) \ge 1$. Then $e(G_1) = 1$, i.e., $C^{(1)}$ is a triangle and the two vertices on $C^{(1)}$ different from u are both of degree two in G. Similarly, $C^{(2)}$ is a triangle and the two vertices on $C^{(2)}$ different from u are both of degree two in G.

Thus G is the bicyclic graph obtained by identifying a vertex of two triangles, and attaching $n - 5$ pendent vertices to the common vertex. By direct calculation, $\mu_1(G) = n$ and $\mu_2(G) = \mu_3(G) = 3$, i.e., $S_3(G) = n + 6 = e(G) + 5$, a contradiction.

Case 3. There are two cycles sharing common edge(s) in G. Note that there are three cycles in G. Let $C^{(1)}$ and $C^{(2)}$ be the two cycles of G such that the remaining one has the maximum length. Let A be the set of the common vertices of $C^{(1)}$ and $C^{(2)}$. Let v_1 and v_2 be the two vertices in A such that the distance from v_1 to v_2 is as large as possible. If there is a non-pendent edge outside the cycles in G, then by Lemma 4.7 (i), $S_3(G) \le e(G) + 6$, a contradiction, and thus every edge outside the cycles of G is a pendent edge.

Denote by v_3 and v_4 the neighbor of v_1 and v_2 in $C^{(1)}$ different from the vertices in A, respectively. Let G_1 be the component of $G - \{v_1v_3, v_2v_4\}$ containing v_3. If $e(G_1) \geq 2$, then by Lemma 4.7 (ii), $S_3(G) \leq e(G) + 6$, a contradiction. Thus $e(G_1) \leq 1$. Denote by v_5 and v_6 the neighbor of v_1 and v_2 in $C^{(2)}$ different from the vertices in A, respectively. Let G_2 be the component of $G - \{v_1v_5, v_2v_6\}$ containing v_5. As above, we have $e(G_2) \leq 1$. If $|A| \geq 3$, then denote by v_7 and v_8 the neighbor of v_1 and v_2 in A, respectively ($v_7 = v_8$ if $|A| = 3$), let G_3 be the component of $G - \{v_1v_7, v_2v_8\}$ containing v_7, and as above, we have $e(G_3) \leq 1$.

Let $n_j = |V(G_j)|$ for $j = 1, 2$ and $n_3 = |V(G_3)|$ if $|A| \geq 3$ and $n_3 = 0$ if $|A| = 2$. Then $n_1 = 1, 2$, $n_2 = 1, 2$, and $n_3 = 0, 1, 2$. By the choice of $C^{(1)}$ and $C^{(2)}$, we have $n_3 \leq \min\{n_1, n_2\}$. Suppose without loss of generality that $n_1 \leq n_2$ and $d_{v_1} \geq d_{v_2}$. If $d_{v_1} \leq 4$, then $n \leq 10$, a contradiction. Thus $d_{v_1} \geq 5$. Let $G' = G - \{v_1v_3, v_1v_5, v_1v_7\}$ if $|A| \geq 3$ and $G' = G - \{v_1v_3, v_1v_5, v_1v_2\}$ if $|A| = 2$. It is easily seen that G' consists of two components, one of which containing v_1, denoted by G_4, is a tree, and the other one containing v_3, denoted by G_5, is also a tree. Let $n_j = |V(G_j)|$ for $j = 4, 5$. Obviously, $G_4 \cong T^0_{n_4}$ with $n_4 \geq 3$, implying that $\mu_1(G_4) = n_4 \geq 3$, $\mu_2(G_4) = 1$. For G_5, we have

$$G_5 \cong \begin{cases} T^0_{n_5} & \text{if } (n_1, n_2, n_3) = (1, 1, 0), (1, 1, 1), \\ T^1_{n_5} & \text{if } (n_1, n_2, n_3) = (1, 2, 0), (1, 2, 1), \\ T^2_{n_5} & \text{if } (n_1, n_2, n_3) = (2, 2, 0), (2, 2, 1), \\ T^3_{n_5} & \text{if } (n_1, n_2, n_3) = (2, 2, 2). \end{cases}$$

If $G_5 \cong T^0_{n_5}$, then the first three largest Laplacian eigenvalues of $G_4 \cup G_5$ are $n_4, n_5, 1$, i.e., $S_3(G_4 \cup G_5) = n + 1$, and thus by Lemma 2.2,

$$\begin{aligned} S_3(G) &\leq S_3(G_4 \cup G_5) + 2 \cdot 3 \\ &= (n + 1) + 6 = e(G) + 6, \end{aligned}$$

a contradiction. If $G_5 \cong T^1_{n_5}$, then $G \in \cup_{i=1}^4 \mathbb{U}^i_n$, and thus by Lemma 4.4, $S_3(G) \leq e(G) + 6$, a contradiction. If $G_5 \cong T^2_{n_5}$ with $n_5 = 5$, then $(n_1, n_2, n_3) = (2, 2, 0)$, implying that $G \cong U^5_n, U^6_n$, or U^7_n, and thus by Lemma 4.4, $S_3(G) \leq e(G) + 6$, a contradiction. Suppose that $G_5 \cong T^2_{n_5}$ with $n_5 \geq 6$, or $G_5 \cong T^3_{n_5}$ with $n_5 \geq 7$. By Lemma 4.6, we have $1 < \mu_2(G_5) < 2.7 < 3 \leq \mu_1(G_4)$, implying that the first three largest Laplacian eigenvalues of $G_4 \cup G_5$ are $\mu_1(G_4) = n_4$, $\mu_1(G_5)$, $\mu_2(G_5)$, i.e., $S_3(G_4 \cup G_5) = n_4 + S_2(G_5)$. By Lemma 4.6, $S_2(G_5) < e(G_5) + 2$. Now it follows from Lemma 2.2 that

$$\begin{aligned} S_3(G) &\leq S_3(G_4 \cup G_5) + 2 \cdot 3 \\ &= (n_4 + S_2(G_5)) + 6 \\ &< (n_4 + e(G_5) + 2) + 6 = e(G) + 6, \end{aligned}$$

a contradiction.

Combining Cases 1–3, there is no counterexample, and thus the result follows. □

By Lemmas 2.4 and 4.8, Proposition 3.5, we have

Corollary 4.2. *Conjecture 1.1 is true for bicyclic graphs.*

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