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Bicyclic graphs with maximum sum of the two largest Laplacian eigenvalues

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Abstract
Let G be a simple connected graph and $S_2(G)$ be the sum of the two largest Laplacian eigenvalues of G. In this paper, we determine the bicyclic graph with maximum $S_2(G)$ among all bicyclic graphs of order n, which confirms the conjecture of Guan *et al.* (J. Inequal. Appl. 2014:242, 2014) for the case of bicyclic graphs.

MSC: 05C50; 15A48

Keywords: Laplacian eigenvalue; largest eigenvalue; sum of eigenvalue; bicyclic graph

1 Introduction

Let $G = (V(G), E(G))$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$. The numbers of its vertices and edges are denoted by $n(G)$ and $m(G)$ (or n and m for short). For a vertex $v \in V(G)$, let $N(v)$ be the set of all neighbors of v in G. The degree of v, denoted by $d(v)$, is the cardinality of $|N(v)|$, that is, $d(v) = |N(v)|$. A vertex with degree one is called pendant vertex. Particularly, denote by $\Delta(G)$ (or Δ for short) the maximum degree of G. The matrix $L(G) = D(G) - A(G)$ is called *Laplacian* matrix of G, where $A(G)$ is the adjacency matrix of G and $D(G) = \mathrm{diag}(d(v_1), d(v_2), \dots, d(v_n))$ is the diagonal matrix of vertex degrees of G. We use the notation I_n for the identity matrix of order n and denote by $\phi(G, x) = \det(xI_n - L(G))$ the *Laplacian* characteristic polynomial of G. It is well known that $L(G)$ is positive semidefinite and so its eigenvalue are nonnegative real number. The eigenvalues of $L(G)$ are called the *Laplacian* eigenvalues of G and are denoted by $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G)$ (or $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ for short), which are always enumerated in non-increasing order and repeated according to their multiplicity. It is well known that $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. Note that each row sum of $L(G)$ is 0 and, therefore, $\mu_n(G) = 0$. Fiedler [2] showed that the second smallest eigenvalue $\mu_{n-1}(G)$ of $L(G)$ is 0 if and only if G is disconnected. Thus the second smallest eigenvalue of $L(G)$ is popularly known as the algebraic connectivity of G. The largest eigenvalue $\mu_1(G)$ of $L(G)$ is usually called the *Laplacian* spectral radius of the graph G. The investigation of Laplacian spectra of graphs is an interesting topic on which much literature focused in the last two decades (see [2–9]).

Let $S_k(G) = \sum_{i=1}^{i=k} \mu_i(G)$ be the sum of the k largest *Laplacian* eigenvalues of G. Hamers in [10] mentions that Brouwer conjectured that $S_k(G) \leq m(G) + \binom{k+1}{2}$ for $k = 1, 2, \dots, n$. This conjecture is interesting and still open. Up to now, little progress on it has been made (see [1, 10–13]). When $k = 2$, Haemers *et al.* [10] proved the conjecture by showing $S_2(G) \leq$

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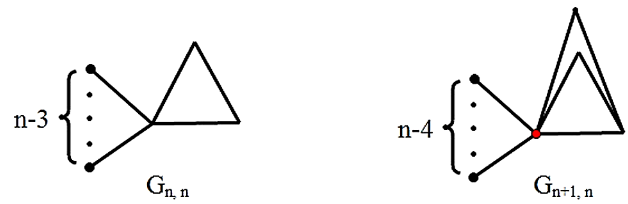


Figure 1 $G_{n,n}$ **and** $G_{n+1,n}$**.**

$m(G) + 3$ for any graph G. Especially when G is a tree, Fritscher *et al.* [14] improve this bound by showing $S_2(T) \leq m(T) + 3 - \frac{2}{n(T)}$, which indicates that Haemers' bound is always not attainable for trees. Therefore, it is interesting to determine which tree has maximum value of $S_2(T)$ among all trees of order n. Let $S^k_{a,b}$ be the tree of order n obtained from two stars S_{a+1}, S_{b+1} by joining a path of length k between their central vertices. Guan *et al.* [1] proved that $S_2(T) \leq S_2(T^1_{\lceil\frac{n-2}{2}\rceil,\lfloor\frac{n-2}{2}\rfloor})$ for any tree of order $n \geq 4$ and the equality holds if and only if $T \cong T^1_{\lceil\frac{n-2}{2}\rceil,\lfloor\frac{n-2}{2}\rfloor}$. Note that $\mu_1(G) \leq n(G)$ for any graph G of order n. When $2n(G) < m(G) + 3$, it follows that $S_2(G) \leq 2n(G) < m(G) + 3$, which means that Haemers' bound is not attainable. When $2n(G) \geq m(G) + 3$, Guan *et al.* [1] showed that $S_2(G_{m,n}) = m(G_{m,n}) + 3$, where $G_{m,n}$ is a graph with n vertices and m edges which has $m - n + 1$ triangles with a common edge and $2n - m - 3$ pendant edges incident with one end vertex of the common edge (illustrated in Figure 1 are $G_{n,n}$ and $G_{n+1,n}$). This indicates that Haemers' bound is always sharp for connected graphs ($n \leq m \leq 2n - 3$). The following conjecture on the uniqueness of the extremal graph is also presented in [1].

Conjecture 1.1 ([1]) *Among all connected graphs with n vertices and m edges* ($n \leq m \leq 2n - 3$), $G_{m,n}$ *is the unique graph with maximal value of* $S_2(G)$, *that is,* $S_2(G_{m,n}) = m(G_{m,n}) + 3$.

Zheng *et al.* [15] determined the uicyclic graph with maximum $S_2(G)$ among all uicyclic graphs of order n, which confirms Conjecture 1.1 for $m = n$.

Theorem 1.2 ([15]) *For any unicyclic graph G of order n,* $S_2(G) \leq m(G) + 3$ *with equality if and only if* $G \cong G_{n,n}$.

In this paper, we prove that Conjecture 1.1 holds for $m = n + 1$. The main result is as follows.

Theorem 1.3 *For any bicyclic graph G of order n,* $S_2(G) \leq m(G) + 3$ *with equality if and only if* $G \cong G_{n+1,n}$.

In Section 2 of this paper, we give some well known lemmas which are useful in the proof of Theorem 1.3. In Section 3, we will give the proof of Theorem 1.3.

2 Preliminaries

We first present some well-known results on $\mu_1(G)$.

Lemma 2.1 ([3]) *Let G be a connected graph of order n, then* $\mu_1(G) \leq n(G)$ *with equality if and only if the complement of G is disconnected.*

Lemma 2.2 ([8]) *Let G be a connected graph of order n, $d_i = d(v_i)$ and $m_i = \sum_{v_j \in N(v_i)} d_j/d_i$. Then*

$$\mu_1(G) \leq \max\{d_i + m_i \mid v_i \in V(G)\}.$$

Lemma 2.3 ([7]) *Let G be a connected graph with $n \geq 4$ vertices and m edges. Then*

$$\mu_1(G) < \max\left\{\triangle(G), m - \frac{n-1}{2}\right\} + 2.$$

Let M be a real symmetric matrix of order n. Then all eigenvalues of M are real and can be denoted by $\lambda_1(M) \geq \lambda_2(M) \geq \cdots \geq \lambda_n(M)$ in non-increasing order. The following result in matrix theory plays a key role in our proofs.

Lemma 2.4 ([16]) *Let A and B be two real symmetric matrices of order n. Then, for any $1 \leq k \leq n$,*

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

The next lemma follows from Lemma 2.4 immediately.

Lemma 2.5 *Suppose $G_1, \ldots, G_r$ are edge disjoint graphs. Then, for any k,*

$$S_k(G_1 \cup \cdots \cup G_r) \leq \sum_{i=1}^{r} S_k(G_i).$$

The following lemma can be found in [17] and is known as the interlacing theorem of Laplacian eigenvalues.

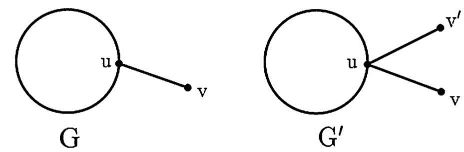
Lemma 2.6 ([17]) *Let G be a graph of order n and G' be the graph obtained from G by deleting an edge of G. Then the Laplacian eigenvalues of G and G' interlace, that is,*

$$\mu_1(G) \geq \mu_1(G') \geq \mu_2(G) \geq \cdots \geq \mu_{n-1}(G') \geq \mu_n(G) \geq \mu_n(G') = 0.$$

Lemma 2.7 ([17]) *Let A be a real symmetric matrix of order n with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and B be a principal submatrix of A of order m with eigenvalues $\lambda'_1 \geq \lambda'_2 \geq \cdots \geq \lambda'_m$. Then the eigenvalues of B interlace the eigenvalues of A, that is, $\lambda_i \geq \lambda'_i \geq \lambda_{n-m+i}$, for $i = 1, \ldots, m$. Specially, for $v \in V(G)$, let $L_v(G)$ be the principal submatrix of $L(G)$ formed by deleting the row and column corresponding to vertex v. Then the eigenvalues of $L_v(G)$ interlace the eigenvalues of $L(G)$.*

The multiplicities of an eigenvalue λ for $L(G)$ is denoted by $m_G(\lambda)$. For a graph G of order n, it is well known that $m_G(1) = n - r(I_n - L(G))$, where $r(I_n - L(G))$ is the rank of $I_n - L(G)$.

Figure 2 Graphs G' and G.



Lemma 2.8 *Let v be a pendant vertex of graph G with n vertices and G' be the graph obtained from G by adding a new vertex v' which has a unique neighbor u, where u is the neighbor of v. (See Figure 2.) Then*

$$m_{G'}(1) = m_G(1) + 1.$$

Proof Let $L(G)$ and $L(G')$ be the Laplacian matrix of G and G', respectively. It is not difficult to check that $r(I_n - L(G)) = r(I_{n+1} - L(G'))$. Thus the result follows from the facts that $m_G(1) = n - r(I_n - L(G))$ and $m_{G'}(1) = (n+1) - r(I_{n+1} - L(G'))$. □

Let P_n and C_n be the path and cycle of order n, respectively. A connected graph with n vertices and $n+1$ edges is called a bicyclic graph. Let $\mathcal{B}_n$ be the set of bicyclic graphs of order n. There are two basic bicyclic graphs: ∞-graph and θ-graph. More concisely, an ∞-graph, denoted by $\infty(p,q,l)$-graph, is obtained from two vertex-disjoint cycles C_p and C_q by connecting one vertex of C_p and one vertex of C_q with a path P_{l+1} of length l, where $q \geq p \geq 3$ and $l \geq 0$ (in the case of $l = 0$, we identify the above two vertices). A θ-graph, denoted by $\theta(p,q,l)$, is a union of three internally disjoint paths P_p, P_q, P_l of length $p-1$, $q-1$, $l-1$, respectively with common end vertices, where $l \geq q \geq p \geq 2$ and at most one of them is 2. Observe that any bicyclic graph G is obtained from a basic bicyclic graph $\infty(p,q,l)$ or $\theta(p,q,l)$ by attaching trees to some of its vertices. For any bicyclic graph G, we call its basic bicyclic graph $\infty(p,q,l)$ or $\theta(p,q,l)$ the kernel of G. For a vertex v of the kernel of G, if there is a tree T_v attached to it, we denote by $e(v)$ the maximum distance between v and any vertex of T_v (that is, $e(v) = \max\{d(u,v) \mid u \in V(T_v)\}$); if there is no tree attached to it, we define $e(v) = 0$. Let $\mathcal{B}_n^{\infty}(p,q,l)$ and $\mathcal{B}_n^{\theta}(p,q,l)$ be the sets of bicyclic graphs of order n with $\infty(p,q,l)$ and $\theta(p,q,l)$ as their kernel, respectively. Clearly, $\mathcal{B}_n = \mathcal{B}_n^{\infty}(p,q,l) \cup \mathcal{B}_n^{\theta}(p,q,l)$. Let S be a multiset of some nonnegative integers, denote by $\|S\|$ the number of nonzero elements in S, that is, $\|S\| = |\{a \in S \mid a \geq 1\}|$, where elements are counted according to their multiplicity.

Lemma 2.9 *Let G be the union of some disjoint graphs $G_1, G_2, \ldots, G_r$, where G_i ($i \in \{1, \ldots, r\}$) is a tree or an unicyclic graph of order n_i which is not isomorphic to G_{n_i,n_i} ($G_{n,n}$ is the unicyclic graph shown in Figure 1). Then $S_2(G) < m(G) + 3$.*

Proof By Theorem 1.2 and the fact $S_2(T) < m(T) + 3$ for any tree, we have $S_2(G_i) < m(G_i) + 3$ for $i \in \{1, \ldots, r\}$. If μ_1 and μ_2 of G attain the same component, say G_{i_0} ($1 \leq i_0 \leq r$), then $S_2(G) = S_2(G_{i_0}) < m(G_{i_0}) + 3 \leq m(G) + 3$. Otherwise, μ_1 and μ_2 of G attain two different components, without loss of generality, we assume that μ_1 and μ_2 attain G_1 and G_2, respectively, that is, $\mu_1 = \mu_1(G_1)$ and $\mu_2 = \mu_1(G_2)$. Then $S_2(G) = \mu_1(G_1) + \mu_1(G_2) \leq n(G_1) + n(G_2) \leq (m(G_1) + 1) + (m(G_2) + 1) \leq m(G) + 2 < m(G) + 3$. □

For any subgraph H of G, let $G - H$ be the graph obtained from G by deleting all edges from H.

Lemma 2.10 *Let G be a simple graph with at least 4 vertex-disjoint P_2 (or 3 vertex-disjoint P_3) such that $G - 4P_2 = \bigcup G_i$ (or $G - 3P_3 = \bigcup G_i$), where G_i is a tree or an unicyclic graph of order n_i which is not isomorphic to G_{n_i,n_i} ($G_{n,n}$ is the unicyclic graph shown in Figure 1). Then $S_2(G) < m(G) + 3$.*

Proof By direct calculation, we have $S_2(4P_2) = m(4P_2) = 4$ and $S_2(3P_3) = m(3P_3) = 6$. Using Lemmas 2.5 and 2.9, we have $S_2(G) \leq S_2(G - 4P_2) + S_2(4P_2) < (m(G - 4P_2) + 3) + m(4P_2) = m(G) + 3$ (or $S_2(G) \leq S_2(G - 3P_3) + S_2(3P_3) < (m(G - 3P_3) + 3) + m(3P_3) = m(G) + 3$), this completes the proof. □

3 Proof of Theorem 1.3

First of all, using the facts that $S_2(G) \leq m(G) + 3$ for any graph G and that $\mathcal{B}_n = \mathcal{B}_n^{\infty}(p,q,l) \cup \mathcal{B}_n^{\theta}(p,q,l)$, we give the main idea of the proof.

1. For each class, we show that $S_2(G) < m(G) + 3$ for the majority of graphs of $\mathcal{B}_n^{\infty}(p,q,l)$ or $\mathcal{B}_n^{\theta}(p,q,l)$ by Lemma 2.10.
2. For the remaining graphs in $\mathcal{B}_n^{\infty}(p,q,l)$ or $\mathcal{B}_n^{\theta}(p,q,l)$ (except for $G_{n+1,n}$), we prove that $S_2(G) < m(G) + 3$ by discussing case by case.
3. We show that $S_2(G_{n+1,n}) = m(G_{n+1,n}) + 3$, that is, the condition that equality holds.

Next, we discuss according to the following two subsections.

3.1 Bicyclic graphs in $\mathcal{B}_n^{\infty}(p,q,l)$

In this subsection, we prove that $S_2(G) < m(G) + 3$ for $G \in \mathcal{B}_n^{\infty}(p,q,l)$.

Lemma 3.1 *Let $G \in \mathcal{B}_n^{\infty}(p,q,l)$. If (p,q,l) satisfies one of the following conditions:*

(1) $l \geq 1$,
(2) $(p,q,l) = (p,q,0)$ *and* $q \geq p \geq 4$,
(3) $(p,q,l) = (3,q,0)$ *and* $q \geq 5$,

then $S_2(G) < m(G) + 3$.

Proof Direct calculation shows that $S_2(C_p \cup C_q) \leq m(C_p \cup C_q)$, where $q \geq p \geq 3$. For (1) $l \geq 1$, using Lemmas 2.5 and 2.9, we have $S_2(G) \leq S_2(G - C_p - C_q) + S_2(C_p \cup C_q) < (m(G - C_p - C_q) + 3) + m(C_p \cup C_q) = m(G) + 3$, since each component of $G - C_p - C_q$ is tree. For both (2) and (3), it is not difficult to check that G has 4 vertex-disjoint P_2 (or 3 vertex-disjoint P_3) such that each component of $G - 4P_2$ (or $G - 3P_3$) is a tree. Thus the result follows from Lemma 2.10. □

By Lemma 3.1, it suffices to consider the following two cases: $G \in \mathcal{B}_n^{\infty}(3,4,0)$ and $G \in \mathcal{B}_n^{\infty}(3,3,0)$.

Lemma 3.2 *For $G \in \mathcal{B}_n^{\infty}(3,4,0)$, we have $S_2(G) < m(G) + 3$.*

Proof For $G \in \mathcal{B}_n^{\infty}(3,4,0)$, its kernel is $\infty(3,4,0)$, denoted by G_1^0 for short shown in Figure 3. Let $V(G_1^0) = \{v_1, \ldots, v_6\}$. If there exists a vertex $v_i \in V(G_1^0)$ such that $e(v_i) \geq 2$, then G has 4 vertex-disjoint P_2 such that each component of $G - 4P_2$ is a tree and the result follows from Lemma 2.10. Thus it suffices to consider the case that G is isomorphic to G_1 shown in Figure 3.

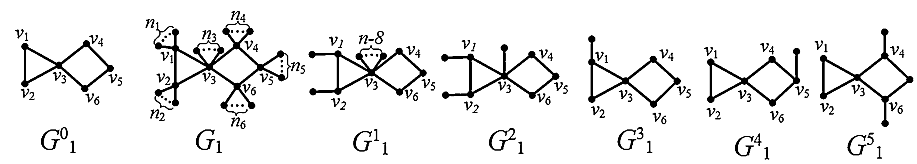


Figure 3 Some bicyclic graphs with $\infty(3,4,0)$ as their kernel.

When $\|\{n_1,n_2,\dots,n_6\}\| \geq 3$, if G is not isomorphic to G_1^1 shown in Figure 3, then G has 4 vertex-disjoint P_2 (or 3 vertex-disjoint P_3) such that each component of $G-4P_2$ (or $G-3P_3$) is a tree or a unicyclic graph of order n_i which is not isomorphic to G_{n_i,n_i}. Thus the result follows from Lemma 2.10. If G is isomorphic to G_1^1, then we have $m_G(1) \geq n-9$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_8 > \lambda_9 = 0$ be the other night eigenvalues of G. Then we have $\lambda_1+\lambda_2+\cdots+\lambda_9 = n+11$, since $\sum_{i=1}^{i=n}\mu_i = 2m(G)$. By Lemma 2.6 and direct calculations, we have $\lambda_3+\lambda_4+\lambda_5 \geq \mu_3(G_1^2)+\mu_4(G_1^2)+\mu_5(G_1^2) = 3.22+2.22+2.00 > 7$, since G_1^1 contains G_1^2 shown in Figure 3 as a subgraph. Therefore $S_2(G) = \lambda_1+\lambda_2 < n+4 = m(G)+3$.

If $\|\{n_1,n_2,\dots,n_6\}\| = 2$, then we have $m_G(1) \geq n-8$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_7 > \lambda_8 = 0$ be the other eight eigenvalues of G. Then we have $\lambda_1+\lambda_2+\cdots+\lambda_8 = n+10$, since $\sum_{i=1}^{i=n}\mu_i = 2m(G)$.

When $n_3 = 0$, G contains a subgraph isomorphic to G_1^i ($i \in \{3,4,5\}$) shown in Figure 3. By Lemma 2.6 and direct calculations, we have $\lambda_3+\lambda_4+\lambda_5 \geq \mu_3(G_1^i)+\mu_4(G_1^i)+\mu_5(G_1^i) > 6$ for $i \in \{3,4,5\}$. Therefore $S_2(G) = \lambda_1+\lambda_2 < n+4 = m(G)+3$.

When $n_3 \geq 1$, it can be checked that $m_G(1) \geq n-7$ by direct calculation and Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_6 > \lambda_7 = 0$ be the other seven eigenvalues of G. Then we have $\lambda_1+\lambda_2+\cdots+\lambda_7 = n+9$, since $\sum_{i=1}^{i=n}\mu_i = 2m(G)$. By Lemma 2.6 and direct calculations, we have $\lambda_3+\lambda_4 \geq \mu_3(G_1^0)+\mu_4(G_1^0) = 5$, since G_1 contains G_1^0 as a subgraph. Therefore $S_2(G) = \lambda_1+\lambda_2 < n+4 = m(G)+3$.

If $\|\{n_1,n_2,\dots,n_6\}\| = 1$, then we have $m_G(1) \geq n-7$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_6 > \lambda_7 = 0$ be the other seven eigenvalues of G. Then we have $\lambda_1+\lambda_2+\cdots+\lambda_7 = n+9$, since $\sum_{i=1}^{i=n}\mu_i = 2m(G)$. By Lemma 2.6 and direct calculation, we have $\lambda_3+\lambda_4 \geq \mu_3(G_1^0)+\mu_4(G_1^0) = 5$, since G contains G_1^0 as a subgraph. Therefore $S_2(G) = \lambda_1+\lambda_2 < n+4 = m(G)+3$.

If $\|\{n_1,n_2,\dots,n_6\}\| = 0$, then G is isomorphic to G_1^0. Direct calculation shows that $S_2(G) < m(G)+3$.

The proof is completed. □

Lemma 3.3 *For $G \in \mathcal{B}_n^\infty(3,3,0)$, we have $S_2(G) < m(G)+3$.*

Proof For $G \in \mathcal{B}_n^\infty(3,3,0)$, its kernel is $\infty(3,3,0)$, denoted by G_2^0 for short shown in Figure 4. Let $V(G_2^0) = \{v_1,\dots,v_5\}$. If there exists a vertex $v_i \in V(G_2^0)$ such that $e(v_i) \geq 2$, then it suffices to consider the case that G is isomorphic to G_2^1 or G_2^2 shown in Figure 4, otherwise G has 4 vertex-disjoint P_2 such that each component of $G-4P_2$ is a tree and the result follows from Lemma 2.10.

When G is isomorphic to G_2^i ($i \in \{1,2\}$), we have $m_G(1) \geq n-7$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_6 > \lambda_7 = 0$ be the other seven eigenvalues of G. Then we have $\lambda_1+\lambda_2+\cdots+\lambda_7 = n+9$, since $\sum_{i=1}^{i=n}\mu_i = 2m(G)$. By Lemma 2.6 and direct calculations we have $\lambda_3+\lambda_4+\lambda_5 \geq$

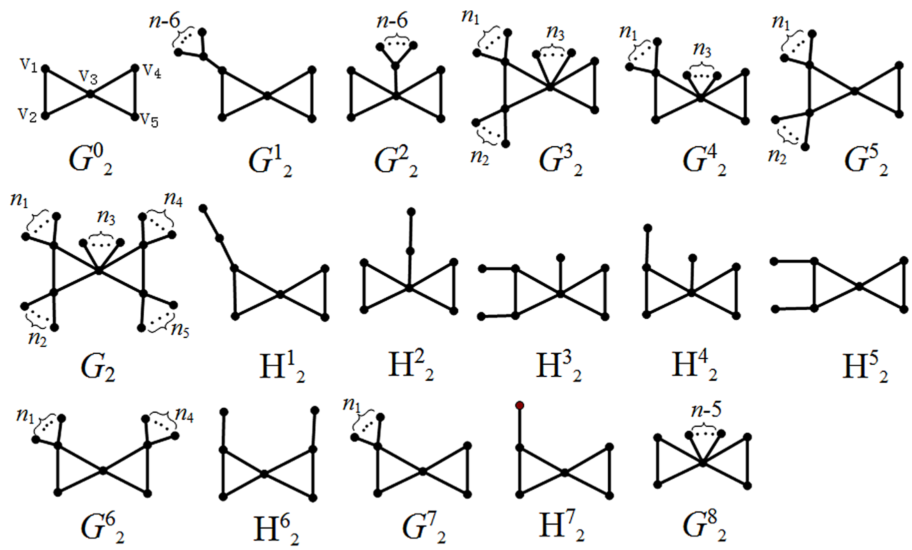


Figure 4 Some bicyclic graphs with $\infty(3,3,0)$ as their kernel.

$\mu_3(H_2^i) + \mu_4(H_2^i) + \mu_5(H_2^i) > 6$, where H_2^i ($i \in \{1,2\}$) is a subgraph of G_2^i shown in Figure 4. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$.

Now, it suffices to consider the case that G is isomorphic to G_2 shown in Figure 4.

When $\|\{n_1, n_2, \dots, n_5\}\| \geq 3$, if G is isomorphic to G_2^3 shown in Figure 4, then G has 4 vertex-disjoint P_2 (or 3 vertex-disjoint P_3) such that each component of $G - 4P_2$ (or $G - 3P_3$) is a tree and the result follows from Lemma 2.10. If G is isomorphic to G_2^3, we have $m_G(1) \geq n - 7$ by direct calculation and Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_6 > \lambda_7 = 0$ be the other seven eigenvalues of G. We have $\lambda_1 + \lambda_2 + \cdots + \lambda_7 = n + 9$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. By Lemma 2.6 and direct calculations we have $\lambda_3 + \lambda_4 \geq \mu_3(H_2^3) + \mu_4(H_2^3) = 3.00 + 2.33 > 5$, where H_2^3 is a subgraph of G shown in Figure 4. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$.

When $\|\{n_1, n_2, \dots, n_5\}\| = 2$, it suffices to consider the case that G is isomorphic to G_2^i ($i \in \{4,5,6\}$) shown in Figure 4. When G is isomorphic to G_2^4, we have $m_G(1) \geq n - 6$ by direct calculation and Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_5 > \lambda_6 = 0$ be the other six eigenvalues of G. We have $\lambda_1 + \lambda_2 + \cdots + \lambda_6 = n + 8$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. By Lemma 2.6 and direct calculations we have $\lambda_3 + \lambda_4 \geq \mu_3(H_2^4) + \mu_4(H_2^4) = 3.00 + 1.51 > 4$, where H_2^4 shown in Figure 4 is a subgraph of G. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$. When G is isomorphic to G_2^i ($i \in \{5,6\}$), we have $m_G(1) \geq n - 7$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_6 > \lambda_7 = 0$ be the other seven eigenvalues of G. Then we have $\lambda_1 + \lambda_2 + \cdots + \lambda_7 = n + 9$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. By Lemma 2.6 and direct calculations we have $\lambda_3 + \lambda_4 \geq \mu_3(H_2^i) + \mu_4(H_2^i) > 5$, where H_2^i shown in Figure 4 is a subgraph of G_2^i. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$.

If $\|\{n_1, n_2, \dots, n_5\}\| = 1$, then it suffices to consider the case that G is isomorphic to G_2^7 or G_2^8 shown in Figure 4. When G is isomorphic to G_2^7, we have $m_G(1) \geq n - 6$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_5 > \lambda_6 = 0$ be the other six eigenvalues of G. We have $\lambda_1 + \lambda_2 + \cdots + \lambda_6 = n + 8$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. By Lemma 2.6 and direct calculations we have $\lambda_3 + \lambda_4 \geq \mu_3(H_2^7) + \mu_4(H_2^7) = 3.00 + 1.4 > 4$, where H_2^7 shown in Figure 4 is a subgraph of G_2^7. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$. When G is isomorphic to G_2^8, by an elementary calculation, we have $\phi(G_2^8,\lambda) = \lambda(\lambda-1)^{n-4}(\lambda-3)^2(\lambda-n)$. It follows that $S_2(G_2^8) = n+3 < m+3$.

If $\|\{n_1,n_2,\dots,n_5\}\| = 0$, then G is isomorphic to G_2^0. Direct calculation shows that $S_2(G) < m(G)+3$. □

We safely come to the following result by the above discussion.

Theorem 3.4 *For $G \in \mathcal{B}_n^{\infty}(p,q,l)$, where $q \ge p \ge 3$ and $l \ge 0$, we have $S_2(G) < m(G)+3$.*

3.2 Bicyclic graphs in $\mathcal{B}_n^{\theta}(p,q,l)$

In this subsection, we prove that $S_2(G) \le m(G)+3$ for $G \in \mathcal{B}_n^{\theta}(p,q,l)$ and equality holds if and only if $G \cong G_{n+1,n}$. We begin with the following lemma, which follows from Lemma 2.10 immediately.

Lemma 3.5 *For $G \in \mathcal{B}_n^{\theta}(p,q,l)$, if (p,q,l) satisfies one of the following conditions:*

(1) $4 \le p \le q \le l$,

(2) $(p,q,l) = (3,q,l)$ *and* $4 \le q \le l$,

(3) $(p,q,l) = (3,3,l)$ *and* $5 \le l$,

then $S_2(G) < m(G)+3$.

By Lemma 3.5, it suffices to consider the following three cases: (1) $G \in \mathcal{B}_n^{\theta}(3,3,4)$, (2) $G \in \mathcal{B}_n^{\theta}(3,3,3)$, and (3) $G \in \mathcal{B}_n^{\theta}(2,q,l)$, where $l \ge q \ge 3$.

First, we consider the case $G \in \mathcal{B}_n^{\theta}(3,3,4)$.

Lemma 3.6 *For $G \in \mathcal{B}_n^{\theta}(3,3,4)$, we have $S_2(G) < m(G)+3$.*

Proof For $G \in \mathcal{B}_n^{\theta}(3,3,4)$, its kernel is $\theta(3,3,4)$, denoted by G_3^0 for short shown in Figure 5. Let $V(G_3^0) = \{v_1,\dots,v_6\}$. If there exists a vertex v_i of G_3^0 such that $e(v_i) \ge 2$, then G has 4 vertex-disjoint P_2 such that each component of $G-4P_2$ is a tree and the result follows from Lemma 2.10. Thus it suffices to consider the case that G is isomorphic to G_3 shown in Figure 5. For $n(G) \le 8$, it is easy to check that $S_2(G) < m(G)+3$ by a direct calculation. Thus we assume that $n(G) \ge 9$ in the following.

If $\|\{n_1,n_2,\dots,n_6\}\| \ge 3$, then G has 4 vertex-disjoint P_2 (or 3 vertex-disjoint P_3) such that each component of $G-4P_2$ (or $G-3P_3$) is a tree and the result follows from Lemma 2.10.

If $\|\{n_1,n_2,\dots,n_6\}\| \le 2$, then we have $m_G(1) \ge n-8$ by Lemma 2.8. Let $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_7 > \lambda_8 = 0$ be the other eight eigenvalues of G. Then we have $\lambda_1+\lambda_2+\cdots+\lambda_8 = n+10$, since $\sum_{i=1}^{i=n}\mu_i = 2m(G)$. When G is not isomorphic to G_3^1 shown in Figure 5, it contains a

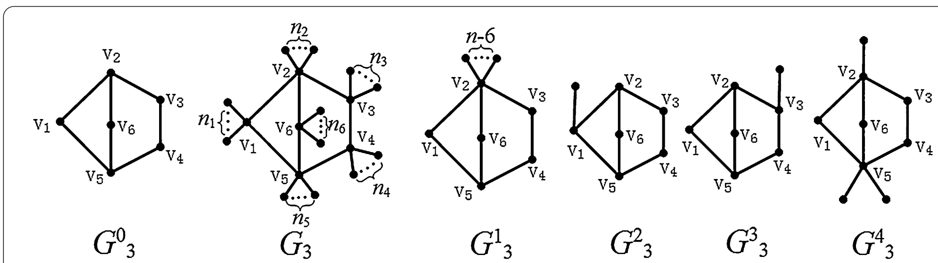


Figure 5 Some bicyclic graphs with $\theta(3,3,4)$ as their kernel.

subgraph which is isomorphic to G_3^i ($i \in \{2,3,4\}$) shown in Figure 5. By Lemma 2.6 and direct calculations, we have $\lambda_3 + \lambda_4 + \lambda_5 \geq \lambda_3(G_3^i) + \lambda_4(G_3^i) + \lambda_5(G_3^i) > 6$ for $i \in \{2,3,4\}$. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n+4 = m(G)+3$. When G is isomorphic to G_3^1, we have $m_G(1) \geq n-7$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_6 > \lambda_7 = 0$ be the other seven eigenvalues of G. Then we have $\lambda_1 + \lambda_2 + \cdots + \lambda_7 = n+9$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. By Lemma 2.6 and direct calculations, we have $\lambda_3 + \lambda_4 + \lambda_5 \geq \mu_3(G_3^0) + \mu_4(G_3^0) + \mu_5(G_3^0) = 2.00 + 2.00 + 1.26 > 5$, since G contains G_3^0 as a subgraph. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n+4 = m(G)+3$.

The proof is completed. □

Second, we consider the case $G \in \mathcal{B}_n^{\theta}(3,3,3)$.

Lemma 3.7 *For $G \in \mathcal{B}_n^{\theta}(3,3,3)$, we have $S_2(G) < m(G)+3$.*

Proof For $G \in \mathcal{B}_n^{\theta}(3,3,3)$, its kernel is $\theta(3,3,3)$, denoted by G_4^0 for short shown in Figure 6. Let $V(G_4^0) = \{v_1,\dots,v_5\}$. If there exists a vertex $v_i \in V(G_4^0)$ such that $e(v_i) \geq 2$, then by Lemma 2.10, it suffices to consider the case that G is isomorphic to G_4^1 or G_4^2 shown in Figure 6.

When G is isomorphic to G_4^1, we have $m_G(1) \geq n-7$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_6 > \lambda_7 = 0$ be the other seven eigenvalues of G. Then we have $\lambda_1 + \lambda_2 + \cdots + \lambda_7 = n+9$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. By Lemma 2.6 and direct calculation, we have $\lambda_3 + \lambda_4 + \lambda_5 \geq \mu_3(H_4^1) + \mu_4(H_4^1) + \mu_5(H_4^1) = 3.00 + 2.00 + 2.00 > 5$, where H_4^1 shown in Figure 6 is a subgraph of G_4^1. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n+4 = m(G)+3$.

When G is isomorphic to G_4^2, we have $m_G(1) \geq n-9$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_8 > \lambda_9 = 0$ be the other nine eigenvalues of G. Then we have $\lambda_1 + \lambda_2 + \cdots + \lambda_9 = n+11$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. If $n_4 \geq 1$ and $n_5 \geq 1$, then G_4^2 contains H_4^2 shown in Figure 6 as a subgraph. By Lemma 2.6 and direct calculations, we have $\lambda_3 + \lambda_4 + \lambda_5 + \lambda_6 \geq \mu_3(H_4^2) + \mu_4(H_4^2) + \mu_5(H_4^2) + \mu_6(H_4^2) = 2.47 + 2.00 + 2.00 + 1.22 > 7$. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n+4 = m(G)+3$. If $n_4 = 0$ or $n_5 = 0$, then we have $m_G(1) \geq n-8$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_7 > \lambda_8 = 0$ be the other eight eigenvalues of G. Then we have $\lambda_1 + \lambda_2 + \cdots + \lambda_8 = n+10$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. By Lemma 2.6 and direct calculation, we have

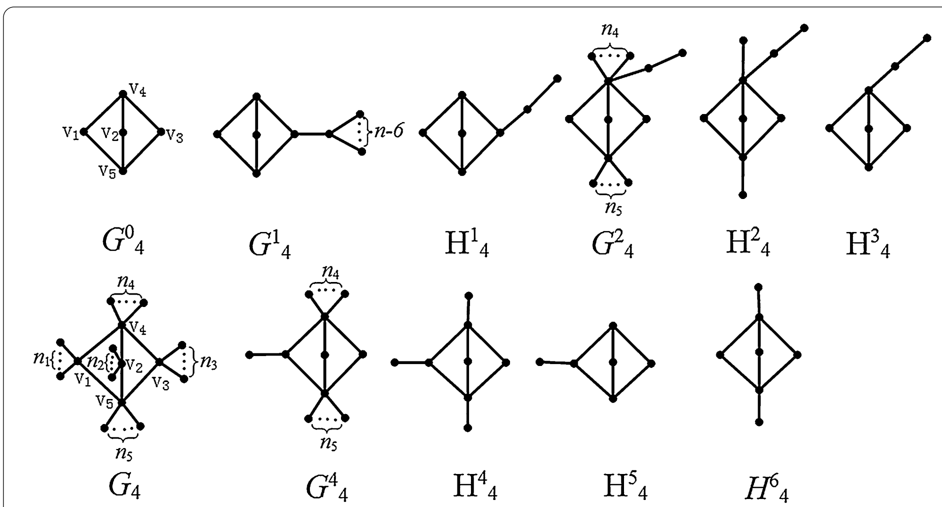


Figure 6 Some bicyclic graphs with $\theta(3,3,3)$ as their kernel.

$\lambda_3 + \lambda_4 + \lambda_5 \geq \mu_3(H_4^3) + \mu_4(H_4^3) + \mu_5(H_4^3) = 2.32 + 2.00 + 2.00 > 6$, where H_4^3 shown in Figure 6 is a subgraph of G_4^2. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$.

Now, we consider the case that G is isomorphic to G_4 shown in Figure 6.

First, we consider the case that $\|\{n_1, n_2, \ldots, n_5\}\| \geq 3$. If G is not isomorphic to G_4^4 shown in Figure 6, then G has 4 vertex-disjoint P_2 (or 3 vertex-disjoint P_3) such that each component of $G - 4P_2$ (or $G - 3P_3$) is a tree and the result follows from Lemma 2.10. When G is isomorphic to G_4^4, we have $m_G(1) \geq n - 8$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_7 > \lambda_8 = 0$ be the other eight eigenvalues of G. Then we have $\lambda_1 + \lambda_2 + \cdots + \lambda_8 = n + 10$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. By Lemma 2.6 and direct calculation, we have $\lambda_3 + \lambda_4 + \lambda_5 \geq \mu_3(H_4^4) + \mu_4(H_4^4) + \mu_5(H_4^4) > 3.08 + 2.00 + 1.29 > 6$, where H_4^4 shown in Figure 6 is a subgraph of G_4^4. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$.

When $\|\{n_1, n_2, \ldots, n_5\}\| = 2$, we have $m_G(1) \geq n - 7$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_6 > \lambda_7 = 0$ be the other seven eigenvalues of G. Then we have $\lambda_1 + \lambda_2 + \cdots + \lambda_7 = n + 9$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. Then by Lemma 2.6 and direct calculations, we have $\lambda_3 + \lambda_4 \geq \mu_3(H_4^i) + \mu_4(H_4^i) \geq 5$ ($i \in \{5, 6\}$), where H_4^i ($i \in \{5, 6\}$) shown in Figure 6 is a subgraph of G. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$.

When $\|\{n_1, n_2, \ldots, n_5\}\| = 1$, we have $m_G(1) \geq n - 6$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_5 > \lambda_6 = 0$ be the other six eigenvalues of G. Then we have $\lambda_1 + \lambda_2 + \cdots + \lambda_6 = n + 8$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. By Lemma 2.6 and direct calculation, we have $\lambda_3 + \lambda_4 \geq \mu_3(G_4^0) + \mu_4(G_4^0) = 2.00 + 2.00 = 4$, since G contains G_4^0 as a subgraph. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$, as required.

When $\|\{n_1, n_2, \ldots, n_5\}\| = 0$, G is isomorphic to G_4^0. Direct calculation shows that $S_2(G) < m(G) + 3$.

From the above discussion, we complete the proof. □

Finally, we consider the case $G \in \mathcal{B}_n^\theta(2, q, l)$, where $l \geq q \geq 3$.

Lemma 3.8 *If $G \in \mathcal{B}_n^\theta(2, q, l)$ with $l \geq q \geq 4$, then $S_2(G) < m(G) + 3$.*

Proof If $q \geq 5$, it is obviously that G has 4 vertex-disjoint P_2 such that $G - 4P_2$ is a forest and the result follows immediately from Lemma 2.10. When $q = 4$ and $l \geq 5$, the result follows immediately from Lemma 2.10, since G has 4 vertex-disjoint P_2 such that $G - 4P_2$ is a forest. Thus it suffices to consider the case that $G \in \mathcal{B}_n^\theta(2, 4, 4)$.

For $G \in \mathcal{B}_n^\theta(2, 4, 4)$, its kernel is $\theta(2, 4, 4)$, denoted by G_5^0 for short shown in Figure 7. Let $V(G_5^0) = \{v_1, \ldots, v_6\}$. If there exists a vertex $v_i \in V(G_5^0)$ such that $e(v_i) \geq 2$, then G has 4 vertex-disjoint P_2 such that each component of $G - 4P_2$ is a tree and the result follows from Lemma 2.10. Now, it suffices to consider the case that G is isomorphic to G_5 shown in Figure 7.

When $\|\{n_1, n_2, \ldots, n_6\}\| \geq 3$, G has 4 vertex-disjoint P_2 (or 3 vertex-disjoint P_3) such that each component of $G - 4P_2$ (or $G - 3P_3$) is a tree and the result follows from Lemma 2.10.

When $1 \leq \|\{n_1, n_2, \ldots, n_6\}\| \leq 2$, we have $m_G(1) \geq n - 8$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_7 > \lambda_8 = 0$ be the other eight eigenvalues of G. Then we have $\lambda_1 + \lambda_2 + \cdots + \lambda_8 = n + 10$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. If G is not isomorphic to G_5^1 shown in Figure 7, then G contains a subgraph which is isomorphic to G_5^2 shown in Figure 7. By Lemma 2.6 and direct calculation, we have $\lambda_3 + \lambda_4 + \lambda_5 \geq \mu_3(G_5^2) + \mu_4(G_5^2) + \mu_5(G_5^2) = 3.00 + 2.22 + 1.38 > 6$. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$. When G is isomorphic to G_5^1, we have

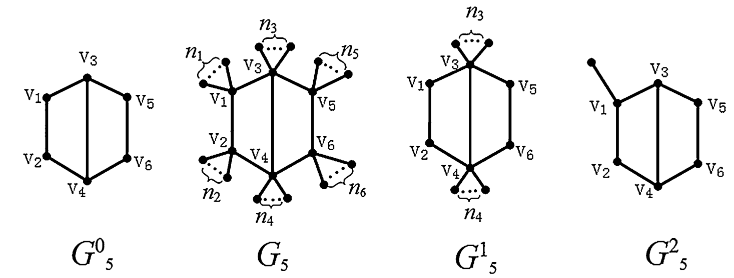


Figure 7 Some bicyclic graphs with $\theta(2,4,4)$ as their kernel.

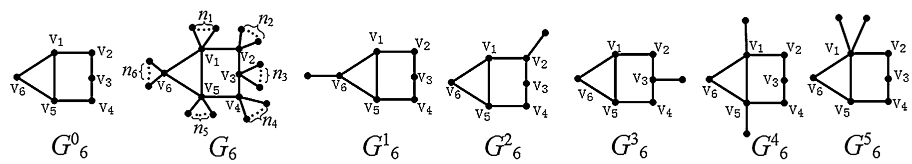


Figure 8 Some bicyclic graphs with $\theta(2,3,5)$ as their kernel.

$m_G(1) = n - 6$ by direct calculation and Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_5 > \lambda_6 = 0$ be the other six eigenvalues of G. Then we have $\lambda_1 + \lambda_2 + \cdots + \lambda_6 = n + 8$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. By Lemma 2.6 and direct calculation, we have $\lambda_3 + \lambda_4 \geq \mu_3(G_5^0) + \mu_4(G_5^0) = 3.00 + 2.00 > 4$, since G_5^1 contains G_5^0 as a subgraph. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$.

When $\|\{n_1, n_2, \ldots, n_6\}\| = 0$, G is isomorphic to G_5^0. Direct calculation shows that $S_2(G) < m(G) + 3$.

The proof is completed. □

Lemma 3.9

If $G \in \mathcal{B}_n^\theta(2,3,l)$ with $l \geq 5$, then $S_2(G) < m(G) + 3$.

Proof When $l \geq 6$, it is obviously that G has 4 vertex-disjoint P_2 such that $G - 4P_2$ is a forest and the result follows immediately from Lemma 2.10. Thus it suffices to consider the case that $G \in \mathcal{B}_n^\theta(2,3,5)$. For $n(G) \leq 7$, it is easy to check that $S_2(G) < m(G) + 3$ by a direct calculation. Thus we assume that $n(G) \geq 8$ in the following.

For $G \in \mathcal{B}_n^\theta(2,3,5)$, its kernel is $\theta(2,3,5)$, denoted by G_6^0 for short shown in Figure 7. Let $V(G_6^0) = \{v_1, \ldots, v_6\}$. If there exists a vertex v_i of G_6^0 such that $e(v_i) \geq 2$, then G has 4 vertex-disjoint P_2 such that $G - 4P_2$ is a forest and the result follows from Lemma 2.10. Now, we can assume that G is isomorphic to G_6 shown in Figure 7.

If $\|\{n_1, n_2, \ldots, n_6\}\| \geq 3$, then G has 4 vertex-disjoint P_2 (or 3 vertex-disjoint P_3) such that each component of $G - 4P_2$ (or $G - 3P_3$) is a tree and the result follows from Lemma 2.10.

If $\|\{n_1, n_2, \ldots, n_6\}\| \leq 2$, then we have $m_G(1) \geq n - 8$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_7 > \lambda_8 = 0$ be the other eight eigenvalues of G. We have $\lambda_1 + \lambda_2 + \cdots + \lambda_8 = n + 10$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. Note that G contains a subgraph which is isomorphic to G_6^i ($i \in \{1,2,3,4,5\}$) shown in Figure 8. By Lemma 2.6 and direct calculations, we have $\lambda_3 + \lambda_4 + \lambda_5 \geq \mu_3(G_6^i) + \mu_4(G_6^i) + \mu_5(G_6^i) > 6$ ($i \in \{1,2,3,4,5\}$). Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$.

The proof is completed. □

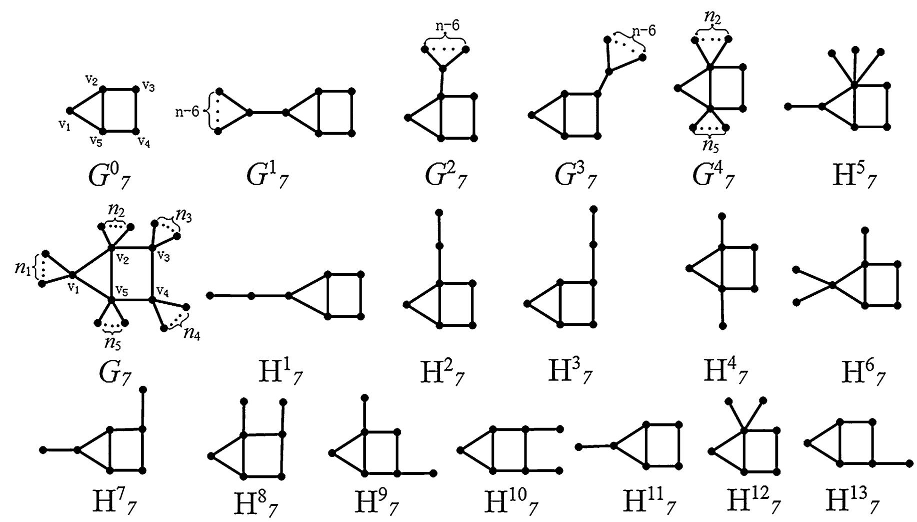


Figure 9 Some bicyclic graphs with $\theta(2,3,4)$ as their kernel.

Lemma 3.10 *For $G \in \mathcal{B}_n^\theta(2,3,4)$, we have $S_2(G) < m(G) + 3$.*

Proof For $G \in \mathcal{B}_n^\theta(2,3,4)$, its kernel is $\theta(2,3,4)$, denoted by G_7^0 for short shown in Figure 9. Let $V(G_7^0) = \{v_1, \ldots, v_5\}$.

If there exists a vertex v_i such that $e(v_i) \geq 2$, then by Lemma 2.10, it suffices to consider the cases that G is isomorphic to G_7^i ($i \in \{1,2,3\}$) shown in Figure 9.

When G is isomorphic to G_7^i ($i \in \{1,2,3\}$) shown in Figure 9, we have $m_G(1) \geq n-7$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_6 > \lambda_7 = 0$ be the other seven eigenvalues of G. We have $\lambda_1 + \lambda_2 + \cdots + \lambda_7 = n + 9$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. By Lemma 2.6 and direct calculations, we have $\lambda_3 + \lambda_4 + \lambda_5 \geq \mu_3(H_7^i) + \mu_4(H_7^i) + \mu_5(H_7^i) > 6$, where H_7^i shown in Figure 9 is a subgraph of G_7^i. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$.

Now, it suffices to consider the case that G is isomorphic to G_7 shown in Figure 9. For $n(G) \leq 8$, it is easy to check that $S_2(G) < m(G) + 3$ by a direct calculation. In the following, we assume that $n(G) \geq 9$.

If $\|\{n_1, n_2, \ldots, n_5\}\| \geq 3$, then G has 4 vertex-disjoint P_2 (or 3 vertex-disjoint P_3) such that each component of $G - 4P_2$ (or $G - 3P_3$) is a tree and the result follows from Lemma 2.10.

If $\|\{n_1, n_2, \ldots, n_5\}\| = 2$, then we have $m_G(1) \geq n - 7$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_6 > \lambda_7 = 0$ be the other seven eigenvalues of G. Then we have $\lambda_1 + \lambda_2 + \cdots + \lambda_7 = n + 9$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. If G is not isomorphic to G_7^4 shown in Figure 9, then it contains a subgraph isomorphic to H_7^i ($i \in \{5, \ldots, 10\}$) shown in Figure 9. By Lemma 2.6 and direct calculations, we have $\lambda_3 + \lambda_4 \geq \mu_3(G_7^i) + \mu_4(G_7^i) > 5$ ($i \in \{5, \ldots, 10\}$). Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$. When G is isomorphic to G_7^4, we have $m_G(1) \geq n - 6$ by direct calculation and Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_5 > \lambda_6 = 0$ be the other six eigenvalues of G. Then we have $\lambda_1 + \lambda_2 + \cdots + \lambda_6 = n + 8$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. By Lemma 2.6 and direct calculations, we have $\lambda_3 + \lambda_4 \geq \mu_3(H_7^4) + \mu_4(H_7^4) > 4$, where H_7^4 shown in Figure 9 is a subgraph of G_7^4. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$.

If $\|\{n_1, n_2, \ldots, n_5\}\| = 1$, then we have $m_G(1) \geq n - 6$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_5 > \lambda_6 = 0$ be the other six eigenvalues of G. Then we have $\lambda_1 + \lambda_2 + \cdots + \lambda_6 = n + 8$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. By Lemma 2.6 and direct calculations, we have $\lambda_3 + \lambda_4 \geq \mu_3(H_7^i) +$

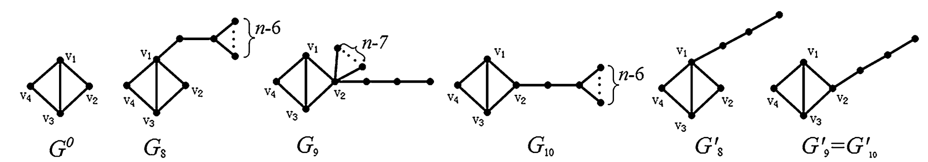


Figure 10 Some bicyclic graphs with $\theta(2,3,3)$ as their kernel.

$\mu_4(H_7^i) > 4$ ($i \in \{11,12,13\}$), where H_7^i shown in Figure 9 is a subgraph of G. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$.

The proof is completed. □

Lemma 3.11 *Let $G \in \mathcal{B}_n^\theta(2,3,3)$ and G^0 shown in Figure* 10 *be the kernel of G. If there exists a vertex v_i of G^0 such that $e(v_i) \geq 3$, then $S_2(G) < m(G) + 3$.*

Proof By Lemma 2.10, it suffices to consider the case that G is isomorphic to G_i ($i \in \{8,9,10\}$) shown in Figure 10.

When G is isomorphic G_i ($i \in \{8,9,10\}$), we have $m_G(1) \geq n - 8$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_7 > \lambda_8 = 0$ be the other eight eigenvalues of G_i. We have $\lambda_1 + \lambda_2 + \cdots + \lambda_8 = n + 10$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. By Lemma 2.6 and direct calculations, we have $\lambda_3 + \lambda_4 + \lambda_5 \geq \mu_3(G_i') + \mu_4(G_i') + \mu_5(G_i') > 6$, where G_i' shown in Figure 10 is the subgraph of G_i. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$.

The proof is completed. □

Lemma 3.12 *Let $G \in \mathcal{B}_n^\theta(2,3,3)$ and G^0 shown in Figure* 10 *be the kernel of G. If $\max_{i=1}^{i=4} e(v_i) = 2$, then $S_2(G) < m(G) + 3$, where v_i is the vertices of G^0.*

Proof By Lemma 2.10, it suffices to consider the case that G is isomorphic to G_{11} or G_{12} shown in Figure 11. Here, we only prove the case that G is isomorphic to G_{11}. For the case G is isomorphic to G_{12}, we can discuss similarly.

When $\|\{n_1, n_2, n_3, n_4\}\| \geq 2$, G has 4 vertex-disjoint P_2 (or 3 vertex-disjoint P_3) such that each component of $G - 4P_2$ (or $G - 3P_3$) is a tree and the result follows from Lemma 2.10.

When $\|\{n_1, n_2, n_3, n_4\}\| \leq 1$, we have $m_G(1) \geq n - 7$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_6 > \lambda_7 = 0$ be the other seven eigenvalues of G. We have $\lambda_1 + \lambda_2 + \cdots + \lambda_7 = n + 9$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. By Lemma 2.6 and direct calculations, we have $\lambda_3 + \lambda_4 \geq \mu_3(G_{11}') + \mu_4(G_{11}') = 3.00 + 2.00 = 5$, where G_{11}' shown in Figure 11 is a subgraph of G_{11}. Thus $S_2(G_{11}) < m(G_{11}) + 3$. □

Lemma 3.13 *Let G_{13} be the bicyclic graph of order n shown in Figure* 12, *where $a \geq b \geq 1$ and $a + b + 5 = n$. Then $S_2(G_{13}) < m(G_{13}) + 3$.*

Proof For $n(G_{13}) \leq 14$, it is easy to check that $S_2(G_{13}) < m(G_{13}) + 3$ by a direct calculation. In following, we assume that $n(G_{13}) \geq 15$.

If $b \geq 5$, then G_{13} contains G_{13}' shown in Figure 12 as a subgraph. Note that $m_{G_{13}}(1) \geq n - 7$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_6 > \lambda_7 = 0$ be the other seven eigenvalues of G_{13}. We have $\lambda_1 + \lambda_2 + \cdots + \lambda_7 = n + 9$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. By Lemma 2.6 and direct calculations, we have $\lambda_3 + \lambda_4 \geq \mu_3(G_{13}') + \mu_4(G_{13}') = 3.197 + 1.810 > 5$. Therefore $S_2(G_{13}) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$.

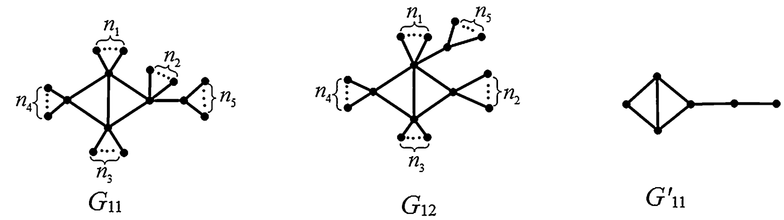


Figure 11 Some bicyclic graphs with $\theta(2,3,3)$ as their kernel.

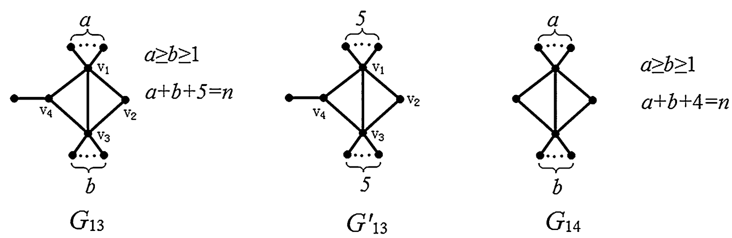


Figure 12 Some bicyclic graphs with $\theta(2,3,3)$ as their kernel.

If $b = 4$, then we have $\lambda_1(G_{13}) < \triangle + 2 = n - 4$ by Lemma 2.3 and $\lambda_2(G_{13}) < \lambda_1(L_{v_1}(G_{13})) = 7.95$ by Lemma 2.7 and direct calculation. It follows that $S_2(G_{13}) < n + 4 = m(G) + 3$.

If $b = 3$, then we have $\lambda_1(G_{13}) < \triangle + 2 = n - 3$ by Lemma 2.3 and $\lambda_2(G_{13}) < \lambda_1(L_{v_3}(G_{13})) = 6.96$ by Lemma 2.7 and direct calculation. It follows that $S_2(G_{13}) < n + 4 = m(G) + 3$.

If $b = 2$, then we have $\lambda_1(G_{13}) < (n - 4) + \frac{n+3}{n-4}$ by Lemma 2.2 and $\lambda_2(G_3) < \lambda_1(L_{v_1}(G_{13})) = 6.005 < 6.10$ by Lemma 2.7 and direct calculation. Therefore $S_2(G_{13}) < n - 4 + \frac{n+3}{n-4} + 6.10 < n + 4 = m(G) + 3$.

If $b = 1$, then we have $\lambda_1(G_{13}) < (n - 3) + \frac{n+3}{n-4}$ by Lemma 2.2 and $\lambda_2(G_{13}) < \lambda_1(L_{v_1}(G_{13})) = 5.10 < 5.20$ by Lemma 2.7 and direct calculation. Thus $S_2(G_{13}) < n - 3 + \frac{n+3}{n-4} + 5.10 < n + 4 = m(G) + 3$. □

Lemma 3.14 *Let G_{14} be the bicyclic graph of order n shown in Figure* 12, *where $a \geq b \geq 1$ and $a + b + 4 = n$. Then $S_2(G_{14}) < m + 3$.*

Proof By some elementary calculations, we have $\phi(G_{14}, x) = x(x - 2)(x - 1)^6 g(x)$, where $g(x) = x^4 - (n + 6)x^3 + (6n + ab + 9)x^2 - (9n + 2ab + 4)x + 4n$. Let $x_1 \geq x_2 \geq x_3 \geq x_4$ be the roots of $g(x) = 0$. Then

$$x_1 + x_2 + x_3 + x_4 = n + 6, \tag{3.1}$$

$$x_1x_2 + x_1x_3 + x_1x_4 + x_2x_3 + x_2x_4 + x_3x_4 = 6n + ab + 9, \tag{3.2}$$

$$x_2x_3x_4 + x_1x_3x_4 + x_1x_2x_4 + x_1x_2x_3 = 9n + 2ab + 4. \tag{3.3}$$

If

$$x_1 + x_2 = n + 4 \tag{3.4}$$

then, by (3.1), we have

$$x_3 + x_4 = 2. \tag{3.5}$$

From (3.2)-(3.5) follows that

$$x_1x_2 + x_3x_4 = 4n + ab + 1, \tag{3.6}$$

$$(n+4)x_3x_4 + 2x_1x_2 = 9n + 2ab + 4. \tag{3.7}$$

By (3.6) and (3.7), we have

$$x_3x_4 = 1. \tag{3.8}$$

Combining (3.5) and (3.8), we have

$$x_3 = x_4 = 1. \tag{3.9}$$

Then $g(1) = -2ab = 0$, which implies that $b = 0$. Therefore, $b \geq 1$ implies that $S_2(G_{14}) < m(G_{14}) + 3$. $\square$

Lemma 3.15 *Let G be the bicyclic graph of order n shown in Figure* 13, *where $a \geq b \geq 0$, $c \geq d \geq 0$ and $a + b + c + d + 4 = n$. Then $S_2(G) \leq m + 3$ with equality if and only if $a = n - 4$ and $b = c = d = 0$ (that is, $G \cong G_{n+1,n}$).*

Proof For $n(G) \leq 12$, it is easy to check that $S_2(G) \leq m(G) + 3$ with equality if and only if $G \cong G_{n+1,n}$ by a direct calculation. In the following, we assume that $n(G) \geq 13$.

When $\|\{a, b, c, d\}\| = 4$, we have $m_G(1) \geq n - 8$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_7 > \lambda_8 = 0$ be the other eight eigenvalues of G. Then we have $\lambda_1 + \lambda_2 + \cdots + \lambda_8 = n + 10$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$.

If $c \geq 2$, then G contains H_1 shown in Figure 12 as a subgraph. By Lemma 2.6 and direct calculations, we have $\lambda_3 + \lambda_4 \geq \mu_3(H_1) + \mu_4(H_1) = 3.94 + 2.14 > 6$. If $c = d = 1$ and $b \geq 2$, then G contains H_2 shown in Figure 12 as a subgraph. By Lemma 2.6 and direct calculations, we have $\lambda_3 + \lambda_4 \geq \mu_3(H_2) + \mu_4(H_2) = 3.414 + 2.593 > 6$. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n + 4 = m(G) + 3$. Now, we can assume that $b = c = d = 1$. Under

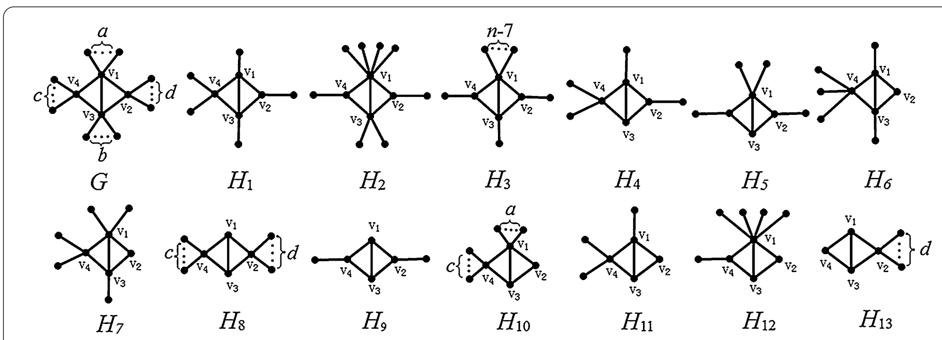


Figure 13 Some bicyclic graphs with $\theta(2,3,3)$ as their kernel.

the assumption, G is isomorphic to H_3 shown in Figure 12. We have $\lambda_1(H_3) < n-2$ by Lemma 2.3 and $\lambda_2(H_3) < \lambda_1(L_{v_1}(H_3)) = 5.23$ by Lemma 2.7 and direct calculation. Therefore, $S_2(G) < (n-2) + 5.23 < n+4 = m(G)+3$.

When $\|\{a,b,c,d\}\| = 3$, we have $m_G(1) \geq n-7$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_6 > \lambda_7 = 0$ be the other seven eigenvalues of G. Then we have $\lambda_1 + \lambda_2 + \cdots + \lambda_7 = n+9$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. If G is isomorphic to G_{13}, then $S_2(G) < m(G)+3$ by Lemma 3.13. Otherwise it contains a subgraph isomorphic to H_i ($i \in \{4,5,6,7\}$) shown in Figure 12. Then we have $\lambda_3 + \lambda_4 \geq \lambda_3(H_i) + \lambda_i(H_i) > 5$ ($i \in \{4,5,6,7\}$) by Lemma 2.6 and direct calculations. Therefore $S_2(G) = \lambda_1 + \lambda_2 < n+4 = m(G)+3$.

When $\|\{a,b,c,d\}\| = 2$, G is isomorphic to G_{14} shown in Figure 12 or H_i ($i \in \{8,10\}$) shown in Figure 12. For G is isomorphic to G_{14}, we have $S_2(G_{14}) < m(G_{14}) + 3$ by Lemma 3.14. For G is isomorphic to H_8 (or H_{10}), we have $m_G(1) \geq n-6$ by Lemma 2.8. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_5 > \lambda_6 = 0$ be the other six eigenvalues of H_8 (or H_{10}). We have $\lambda_1 + \lambda_2 + \cdots + \lambda_6 = n+8$, since $\sum_{i=1}^{i=n} \mu_i = 2m(G)$. Note that H_8 contains H_9 as a subgraph (H_{10} contains H_{11} or H_{12} as a subgraph), where H_i ($i = 9,11,12$) shown in Figure 12. By Lemma 2.6 and direct calculations, we have $\lambda_3 + \lambda_4 \geq \mu_3(H_i) + \mu_4(H_i) > 4$ ($i = 9,11,12$). Therefore $S_2(G) = \lambda_1 + \lambda_2 < n+4 = m(G)+3$, as required. When $\|\{a,b,c,d\}\| = 1$, G is isomorphic to H_{13} or $G_{n+1,n}$. We have $\lambda_1(H_{13}) < n$ by Lemma 2.2 and $\lambda_2(H_{13}) = 4$ by direct calculations. It follows that $S_2(H_{13}) < n+4$. For $G_{n+1,n}$, a direct calculation shows that $S_2(G_{n+1,n}) = m+3$. □

From the discussion above, we safely come to the following result.

Theorem 3.16 *For $G \in \mathcal{B}_n^{\theta}(p,q,l)$, where $l \geq q \geq p \geq 2$ and at most one of them is 2, we have $S_2(G) \leq m(G)+3$ and the equality holds if and only if $G \cong G_{n+1,n}$.*

Theorem 1.3 follows immediately from Theorems 3.4 and 3.16.

Competing interests
The authors declare that they have no competing interests.

Authors' contributions
YRZ carried out the proofs of main results in the manuscript. AC, JXL and SR participated in the design of the study and drafted the manuscripts. All the authors read and approved the final manuscripts.

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