Bicyclic graphs with extremal values of PI index

Žana Kovijanić Vukičević, Dragan Stevanović

Faculty of Natural Sciences and Mathematics, University of Montenegro, Džordža Vušingtona bb, 81000 Podgorica, Montenegro
University of Niš, PMF, Višegradska 33, 18000 Niš, Serbia
University of Primorska, UP IAM, Muzejski trg 2, SI-6000 Koper, Slovenia

Abstract

We give sharp lower and upper bounds on the PI index of connected bicyclic graphs with constant number of vertices and characterize the case of equality for both bounds.

Keywords: Padmakar-Ivan index; Bicyclic graphs.

1. Introduction

Let $G = (V, E)$ be a simple connected graph with $n = |V|$ vertices and $m = |E|$ edges. For each edge $e = (u, v) \in E$, let $m_u(e|G)$ be the number of edges in $G$ lying closer to the vertex $u$ than to the vertex $v$, and similarly, let $m_v(e|G)$ be the number of edges in $G$ lying closer to the vertex $v$ than to the vertex $u$. The Padmakar-Ivan index is defined as

$$PI(G) = \sum_{e=(u,v)\in E} [m_u(e|G) + m_v(e|G)].$$

The Padmakar-Ivan index, abbreviated as PI index, has been proposed in 2000 in [1], its discriminating power in QSAR/QSPR studies was discussed in [2], while its basic mathematical properties have been considered in [3]. The values of PI index for a number of classes of molecular graphs have been obtained in [4]–[15]. The computation of the PI index in partial cubes and benzenoids has been studied in [16, 17], for product graphs it has been obtained in [18], while for bridge and chain graphs it has been given in [19]. A survey of a number of other results and applications of PI index is given in [20].

Another set of questions that attracted attention of researchers are the bounds and the extremal graphs for PI index. It has been shown by Deng

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Supported by the research grants 174033 of the Serbian Ministry of Education and Science and P1-0285 and J1-4021 of the Slovenian Agency for Research.

* Corresponding author.

Email addresses: zanakot-com.me (Žana Kovijanić Vukičević), dragance106@yahoo.com (Dragan Stevanović)

Preprint submitted to Discrete Applied Mathematics September 10, 2012
that \( \text{PI}(G) \geq M_1(G) - 2m \) with equality if and only if \( G \) is a complete multipartite graph, where \( M_1(G) \) is the sum of the squares of the vertex degrees of \( G \), usually referred to as the first Zagreb index of \( G \) [22]. Deng [23] has also shown that, in the class of catacondensed hexagonal systems, the minimum PI index is reached for the linear hexagon chain, while the maximum PI index is obtained for those systems in which each hexagon, apart from the terminal ones, is either angularly connected to two other hexagons or connected to three other hexagons.

However, in the class of all graphs on \( n \)-vertices, it is still an open question which graph attains the maximum PI index. A suggestion of Deng [21] that it may be the complete graph \( K_n \) has been rejected by Khalifeh et al. in [24]. The complete graph \( K_n \) has PI index equal to \( n(n-1)(n-2) \), while Khalifeh et al. constructed a sequence \( H_n \) of graphs satisfying \( \lim_{n \to \infty} \text{PI}(H_n)/n^4 = 5/256. \) Another such sequence of graphs is formed by balanced blown-ups \( B_n \) of a pentagon, obtained by replacing each vertex of \( C_5 \) with a set of either \( \lfloor n/5 \rfloor \) or \( \lceil n/5 \rceil \) vertices, and by replacing each edge of \( C_5 \) with all possible edges between the corresponding sets of vertices (this example appears in an 1984 conjecture of Erdös on the maximum number of pentagons in triangle-free graphs [25]). It is easy to see straight from the definition that \( \lim_{n \to \infty} \text{PI}(B_n)/n^4 = 2/125. \) Khalifeh et al. [24] further conjectured that \( 3/125 \) is the maximum value of a limit of ratios between PI index of a sequence of graphs and \( n^4 \), but without suggesting what graphs constitute such maximum sequence.

When working with graphs having constant number \( m \) of edges, it becomes easier to consider a value that is complementary to PI index. Note that the contribution of each edge \( e = (u,v) \) to \( \text{PI}(G) \) in the formula (1) is the number of edges which are not equidistant from its endpoints \( u \) and \( v \). For the edges \( e = (u,v) \) and \( e' \), let us define

\[
\delta_{e' = (u,v)} = \begin{cases} 
1, & d(u,e') = d(v,e'), \\
0, & d(u,e') \neq d(v,e').
\end{cases}
\]

Then \( \sum_{e' \in E} \delta_e \) is the number of edges that are equidistant to \( u \) and \( v \). (Note that \( \delta_e \neq \delta_{e'} \) may hold for \( e \neq e' \in E \) and that \( \delta_e = 1 \) for each \( e \in E \).) Let us define

\[
S^*(G) = \sum_{e \in E} \sum_{e' \in E} \delta_{e'}.
\]

From (1) it follows that

\[
\text{PI}(G) = \sum_{e \in E} \left[ m - \sum_{e' \in E} \delta_e \right] = m^2 - \sum_{e \in E} \sum_{e' \in E} \delta_{e'} = m^2 - S^*(G). \tag{2}
\]

Hence, the minimum and the maximum of the PI index in the set of graphs with a constant number \( m \) of edges are achieved for those graphs attaining the maximum and the minimum value of \( S^*(G) \), respectively.

Since \( \delta_e = 1 \), we immediately have \( S^*(G) \geq m \), hence, for each \( G \) holds

\[
\text{PI}(G) \leq m(m-1), \tag{3}
\]

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which has been obtained earlier in [3] and [21]. They also proved that equality holds in (3) if and only if \( G \) is either a tree or an odd cycle.

Note that if \( e \) is a cut edge of \( G \), then no edge of \( G \), other than \( e \) itself, can be equidistant to both ends of \( e \) and \( \sum_{e' \in E} \delta_{e'} = 1 \) in such case. Therefore, PI index of every tree has to be equal to \( m(m - 1) \), since its every edge is a cut edge.

Further, if \( G \) is a unicyclic graph, then all of its edges are cut edges, except for the cycle edges. Let \( c \) be the length of a cycle in \( G \). If \( c \) is odd, then for each cycle edge \( e \), the edges equidistant to it (other than \( e \)) belong to a subtree attached to the vertex of a cycle opposite to \( e \). Since each noncycle edge is equidistant to exactly one cycle edge, it follows from (2) that \( PI(G) = m^2 - m - (m - c) \). If \( c \) is even, then for each cycle edge \( e \), the only two edges equidistant to it are \( e \) and the opposite cycle edge. Hence, in this case \( PI(G) = m^2 - m - c \). These questions were further elaborated in [26].

Our goal here is to proceed further to the class of bicyclic graphs with constant number of vertices, obtain sharp lower and upper bounds on their PI index and characterize bicyclic graphs with extremal values of the PI index. Recall that a bicyclic graph is a connected graph having \( |E| = |V| + 1 \) edges. Since the definition of PI index implicitly assumes the graph to be connected, we will assume that all graphs mentioned in the sequel are connected, without explicitly mentioning it.

Let us now define a particular class of bicyclic graphs that will contain our extremal graphs.

**Definition 1.** For \( q, r, s \geq 1 \), let \( P_{q+1}, P_{r+1} \) and \( P_{s+1} \) be the paths of lengths \( q \), \( r \) and \( s \), respectively. Select a left and a right endvertex in each path. The graph \( B_{q,r,s} \) is a bicyclic graph obtained from \( P_{q+1} \cup P_{r+1} \cup P_{s+1} \) by identifying left endvertices as a new vertex \( a \), and by identifying right endvertices as a new vertex \( b \).

Let us introduce some further notation as well:

- for odd \( m \geq 5 \), let \( U_m = B_{2,2,m-4} \);
- for \( m = 3k \geq 6 \), let \( L_{3k} = B_{k,k,k} \);
- for \( m = 3k + 2 \geq 8 \), let \( L_{3k+2} = B_{k,k,k+2} \).

Our main results are the following two theorems.

**Theorem 1.** Let \( G \) be a connected bicyclic graph with \( m \) edges. Then

\[
PI(G) \leq m^2 - m - 4.
\]

The equality is attained if and only if \( m \) is odd and \( G \cong U_m \).

**Theorem 2.** Let \( G \) be a connected bicyclic graph with \( m \) edges. Then

\[
PI(G) \geq \begin{cases} m^2 - 3m, & \text{if } m \equiv 0 \pmod{3}, \\ m^2 - 3m + 2, & \text{if } m \equiv 2 \pmod{3}, \\ m^2 - 3m + 4, & \text{otherwise.} \end{cases}
\]
The equality is attained if and only if \( m \equiv 0, 2 \pmod{3} \) and \( G = L_m \).

Overview of the paper is as follows: detailed discussion of pairs of equidistant edges in bicyclic graphs is spread along the subsections of Section 2, after which we prove Theorem 1 in Section 3 and Theorem 2 in Section 4.

2. Pairs of equidistant edges

Throughout this section, let \( G \) be a connected bicyclic graph with \( m \) edges. We will use \( S^* \) to denote \( S^*(G) \) in the sequel. The cycles of \( G \) may be edge-disjoint or sharing some edges, and we consider these two cases separately.

2.1. The cycles of \( G \) are edge-disjoint

Let \( C' \) and \( C'' \) be the edgesets of the edge-disjoint cycles of \( G \). Then

\[
S^* = \sum_{e \in C'} \sum_{e'} \delta_{e'} + \sum_{e \in C''} \sum_{e'} \delta_{e'} + \sum_{e \in C' \cup C''} \sum_{e'} \delta_{e'}.
\]

Since each edge not belonging to \( C' \cup C'' \) is a cut edge of \( G \), it follows that no edge of \( G \), other than \( e \) itself, can be equidistant to both ends of \( e \). Hence, the contribution to \( S^* \) of each edge not in \( C' \cup C'' \) is equal to 1.

Let \( m' \) be the length of the cycle \( C' \), \( m'' \) the length of the cycle \( C'' \) and \( t = m - m' - m'' \) the number of remaining edges in \( G \). The contribution of an edge \( e \) from \( C' \) depends on the parity of the length of \( C' \): if \( C' \) is even, then the contribution of each edge of \( C' \) to \( S^* \) is equal to 2; if \( C' \) is odd, then the edge opposite to that vertex of \( C' \), which belongs to the path connecting \( C' \) and \( C'' \), contributes to \( S^* \) at least \( m'' + 1 \) and at most \( m - (m' - 1) \), while the contribution of the remaining \( m' - 1 \) edges of \( C' \) to \( S^* \) is equal to 1. Similar argument holds for the edges of \( C'' \). Therefore,

\[
S^* \leq \begin{cases} 
 2m' + 2m'' + t, & C', C'' \text{ even,} \\
 2m' + m + t, & C', C'' \text{ odd,} \\
 m + m + t, & C' \text{ even, } C'' \text{ odd,} \\
 m + m' + t, & C' \text{ odd, } C'' \text{ even.}
\end{cases}
\]

Since \( m = m' + m'' + t \) we get

\[
S^* \leq \max\{3m - m' - m'', 3m - 2m'' - t, 3m - 2m' - t\}. \tag{6}
\]

Since \( m', m'' \geq 3 \), we obtain

**Lemma 3.** If the cycles of a connected bicyclic graph \( G \) are edge-disjoint, then \( S^* \leq 3m - 6 \).

On the other hand, we have

\[
S^* \geq \begin{cases} 
 2m' + 2m'' + t, & C', C'' \text{ even,} \\
 (m'' + 1 + m' - 1) + (m' + 1 + m'' - 1) + t, & C', C'' \text{ odd,} \\
 2m' + (m' + 1 + m'' - 1) + t, & C' \text{ even, } C'' \text{ odd,} \\
 (m'' + 1 + m' - 1) + 2m'' + t, & C' \text{ odd, } C'' \text{ even.}
\end{cases}
\]
Thus
\[ S^* \geq \min\{m + m' + m'', m + 2m', m + 2m''\}. \] (7)

Similarly, from \( m', m'' \geq 3 \), we obtain

**Lemma 4.** If the cycles of a connected bicyclic graph \( G \) are edge-disjoint, then \( S^* \geq m + 6 \).

2.2. The cycles of \( G \) have edges in common

In this case, the union \( C' \cup C'' \) of the edge sets \( C' \) and \( C'' \) of the cycles of \( G \) is isomorphic to \( B_{q,r,s} \). Let \( a \) and \( b \) denote the common end vertices of three paths in \( B_{q,r,s} \). Without loss of generality, suppose that \( q \leq r \leq s \).

2.2.1. Edges equidistant to roots of trees attached to \( B_{q,r,s} \)

Let \( t \) be the number of edges of \( G \) not belonging to \( B_{q,r,s} \), hence, belonging to the set \( T \) of trees obtained by deleting the edges of \( B_{q,r,s} \).

For an arbitrary tree \( T \in \mathcal{T} \), let its root \( w \) be the unique vertex in \( B_{q,r,s} \) belonging to \( T \). Consider in detail the case when \( w \) belongs to the path \( P_{q+1} \), and let us determine the number of edges \( e = (u, v) \) in \( B_{q,r,s} \) that are equidistant to \( w \), i.e., such that \( d(u, w) = d(v, w) \), where \( d(x, y) \) denotes the length of the shortest walk in \( G \) between vertices \( x \) and \( y \). Obviously, the shortest walks \( W_{u,w} \) from \( u \) to \( w \) and \( W_{v,w} \) from \( v \) to \( w \) have to start in opposite directions, \( W_{u,w} \) from \( u \) towards \( a \) and \( W_{v,w} \) from \( v \) towards \( b \), supposing, without loss of generality, that \( a - u - v - b \) is the order of vertices along the path containing \( e \).

First, the case \( e \in P_{q+1} \) is impossible, as the distance from \( w \) to one end vertex of \( e \) along \( P_{q+1} \) will be strictly smaller than \( q \), while the distance from \( w \) to another end vertex across \( P_{r+1} \) (which is the shorter of the paths \( P_{r+1} \) and \( P_{s+1} \)), will be at least \( r \).

Second, if \( e \in P_{r+1} \), then the shortest walk \( W_{u,w} \) will go from \( w \) along \( P_{q+1} \) towards \( a \) and then along \( P_{r+1} \) towards \( u \), while the shortest walk \( W_{v,w} \) will go from \( w \) along \( P_{q+1} \) towards \( b \) and then along \( P_{r+1} \) towards \( v \). Hence, these two shortest walks and the edge \( e \) together form the cycle \( P_{q+1} \cup P_{r+1} \). Since the lengths of the walks \( W_{u,w} \) and \( W_{v,w} \) are supposed to be equal, we conclude that if \( q + r \) is odd, then there exists unique edge \( e \in P_{r+1} \), whose end vertices are equidistant from \( w \); otherwise, no such edge exists.

Third, let \( e \in P_{s+1} \). As the shortest walk \( W_{u,w} \) has to contain \( a \), then, depending on which one is shorter, \( W_{u,w} \) is equal to either the walk from \( w \) to \( a \) along \( P_{q+1} \), followed by the walk from \( a \) to \( u \) along \( P_{s+1} \), or the walk from \( w \) to \( b \) along \( P_{q+1} \), followed by \( P_{r+1} \), and then along \( P_{s+1} \), or the walk form \( w \) to \( a \) along \( P_{q+1} \), followed by \( P_{s+1} \), and then along \( P_{r+1} \). If neither \( W_{u,w} \) nor \( W_{v,w} \) contain \( P_{r+1} \), then the unique edge \( e \in P_{s+1} \) equidistant to \( w \) exists if and only if \( q + s \) is odd. If one of \( W_{u,w} \) and \( W_{v,w} \) contains \( P_{r+1} \), then the unique edge \( e \in P_{s+1} \) equidistant to \( w \) exists if and only if \( r + s \) is odd. The case that both \( W_{u,w} \) and \( W_{v,w} \) contain \( P_{r+1} \) is clearly impossible.
Hence, $B_{q,r,s}$ contains at most two edges equidistant to $w$. If not all of $q, r, s$ have the same parity, then there is always at least one such edge. If all of $q, r, s$ have the same parity, then there are no such edges. In any case, any such edge $e \in B_{q,r,s}$ and each edge $e' \in T$ yield a pair with $\delta'_e = 1$. The same conclusion holds for the other two cases $w \in P_{r+1}$ and $w \in P_{s+1}$, which can be considered analogously.

Let $H$ denote the set of edges in $B_{q,r,s}$ equidistant to the roots of trees in $T$,

$$H = \bigcup_{w \text{ is a root of a tree in } T} \{e = (u,v) \in B_{q,r,s} | d(u,w) = d(v,w)\}.$$ 

From the definition of $H$, we have that

$$\sum_{e \in H} \sum_{e' \notin B_{q,r,s}} \delta'_e = 0.$$ 

Further, from the above discussion we have

**Lemma 5.** If all of $q, r, s$ have the same parity, then

$$\sum_{e \in H} \sum_{e' \notin B_{q,r,s}} \delta'_e = 0. \quad (8)$$

If not all of $q, r, s$ have the same parity, then

$$t = |T| \leq \sum_{e \in H} \sum_{e' \notin B_{q,r,s}} \delta'_e \leq 2|T| = 2t. \quad (9)$$

Further, any edge that does not belong to $B_{q,r,s}$ is a cut edge, hence its contribution to $S^*$ is one and

$$\sum_{e \notin B_{q,r,s}} \sum_{e'} \delta'_e = t.$$ 

Finally, we have that

$$S^* = \sum_{e \in H} \sum_{e' \notin B_{q,r,s}} \delta'_e + \sum_{e \in B_{q,r,s}} \sum_{e' \in B_{q,r,s}} \delta'_e + t, \quad (10)$$

and it remains to estimate the second term in the equation above.

2.2.2. Pairs of equidistant edges in $B_{q,r,s}$.

Now we will determine the pairs of edges $e, e' \in B_{q,r,s}$ satisfying $\delta'_e = 1$. A trivial case of $e = e'$ yields $q + r + s$ such pairs.

Suppose first that $e = (u,v)$ and $e' \neq e$ both belong to the same path $P' \in \{P_{q+1}, P_{r+1}, P_{s+1}\}$. Since the shortest walks $W_{u,e'}$ from $u$ to $e'$ and $W_{v,e'}$ from $v$ to $e'$ have to start in opposite directions from $e$ (otherwise, the lengths of these shortest walks will differ by one and not be equal), one of these walks will
go along $P'$ from an end vertex of $e$ to $e'$, while the other walk (in the case the order along $P'$ is $a - e' - e - b$) will go from another end vertex of $e$ to $b$ along $P'$, then to $a$ along the shorter of the other two paths $\{P_{q+1}, P_{r+1}, P_{s+1}\} \setminus \{P'\}$, and then to $e'$ along $P'$. Therefore, the union of the walks $W_{u,e'}$ and $W_{v,e'}$ of equal length and the edges $e$ and $e'$ forms an even cycle $C$ consisting of $P'$ and the shorter of the two remaining paths. Let the length of $C$ be $2p$. The length of the walk from an end vertex of $e$ to $P'$ is then equal to $p - 1$, and since both $e$ and $e'$ have to belong to $P'$, we see that there are $|P'| - p$ such pairs $(e, e')$ in the case the order along $P'$ is $a - e' - e - b$, and another $|P'| - p$ such pairs in the case the order along $P'$ is $a - e - e' - b$. Surely, if the length of $C$ is odd, no such pair exists. By summing up the cases of $P' = P_{s+1}$, $P' = P_{r+1}$ and $P' = P_{q+1}$ (in which case there are no such pairs $(e, e')$, since, even if $P_{q+1}$ and $P_{r+1}$ do form an even cycle, the term $2(q - \frac{q+1}{2}) = q - r$ is nonpositive), we obtain

**Lemma 6.** The number of pairs $(e, e')$ with $\delta_e = 1$, where $e \neq e'$ belong to the same path in $\{P_{q+1}, P_{r+1}, P_{s+1}\}$ is equal to

$$q + r + s + \begin{cases} r - q, & \text{if } r + q \text{ is even} \\ 0, & \text{if } r + q \text{ is odd} \end{cases} + \begin{cases} s - q, & \text{if } s + q \text{ is even} \\ 0, & \text{if } s + q \text{ is odd} \end{cases}.$$ 

Suppose now that $e = (u, v) \in P$ and $e' \in P'$ belong to different paths $P, P' \in \{P_{q+1}, P_{r+1}, P_{s+1}\}$. Supposing, without loss of generality, that the order along $P$ is $a - u - v - b$, the shortest walks of equal length, $W_{u,e'}$ from $u$ to $e'$ and $W_{v,e'}$ from $v$ to $e'$, have to start in opposite directions: $W_{u,e'}$ will go from $u$ to $a$ along $P$, while $W_{v,e'}$ will go from $v$ to $b$ along $P$. There are now three cases to consider, depending on how the shortest walks continue from there:

(i) the shortest walk $W_{v,e'}$ continues from $b$ towards $a$ along the third path $\{P''\} = \{P_{q+1}, P_{r+1}, P_{s+1}\} \setminus \{P, P'\}$. This is possible only if $P''$ is strictly shorter than $P'$ and, moreover, only if the length of the path $P''$ together with the length of the part of $P'$ from $a$ to $e'$ is strictly smaller than the part of $P'$ from $b$ to $e'$. Then the shortest walks $W_{u,e'}$ and $W_{v,e'}$ share the parts from $a$ to $e'$ along $P'$, while the part of $W_{u,e'}$ from $u$ to $a$, the part of $W_{v,e'}$ from $v$ to $a$ and the edge $e$ form an odd cycle $C' = P \cup P''$. Let the length of the cycle $C'$ be $2p + 1$. Then the walk from $u$ to $a$ along $P$ has length $p$, hence the path $P$ has length at least $p + 1$, and we conclude that also $P$ has to be strictly longer than $P''$. Therefore, it has to be $P'' = P_{q+1}$, while $(P, P') = (P_{r+1}, P_{s+1})$ or $(P, P') = (P_{s+1}, P_{r+1})$. In any case, the choice of $e$ is unique, while $e'$ can be chosen among the first $\lceil (|P'| - |P''|)/2 \rceil$ edges starting from $a$ along the path $P'$. To conclude, the number of pairs $(e, e')$ with $\delta_e = 1$ in this case is equal to

$$\begin{cases} \lfloor (s - q)/2 \rfloor, & \text{if } r + q \text{ is odd} \\ 0, & \text{if } r + q \text{ is even} \end{cases} + \begin{cases} \lfloor (r - q)/2 \rfloor, & \text{if } s + q \text{ is odd} \\ 0, & \text{if } s + q \text{ is even} \end{cases}.$$
(ii) the shortest walk \( W_{u,e'} \) continues from \( a \) towards \( b \) along the third path \( \{P''\} = \{P_{q+1}, P_{r+1}, P_{s+1}\} \setminus \{P, P'\} \). This case is analogous to the previous case and we conclude that the number of pairs \((e, e')\) with \( \delta_{e'} = 1 \) in this case is equal to

\[
\left\{ \begin{array}{ll}
\lfloor (s - q)/2 \rfloor, & \text{if } r + q \text{ is odd} \\
0, & \text{if } r + q \text{ is even}
\end{array} \right. + \left\{ \begin{array}{ll}
\lfloor (r - q)/2 \rfloor, & \text{if } s + q \text{ is odd} \\
0, & \text{if } s + q \text{ is even}
\end{array} \right.
\]

(iii) the shortest walk \( W_{u,e'} \) continues from \( a \) towards \( e' \) along \( P'' \), while the shortest walk \( W_{v,e'} \) continues from \( b \) towards \( e' \) along \( P' \). This case is feasible only if

(a) the sum of the lengths of the third path \( \{P''\} = \{P_{q+1}, P_{r+1}, P_{s+1}\} \setminus \{P, P'\} \) and the part of \( P' \) from \( b \) to \( e' \) is greater than or equal to the length of the part of \( P'' \) from \( a \) to \( e' \), and

(b) the sum of the lengths of \( P'' \) and the part of \( P' \) from \( a \) to \( e' \) is greater than or equal to the length of the part of \( P'' \) from \( b \) to \( e' \).

The equal length walks \( W_{u,e'} \) and \( W_{v,e'} \), together with the edges \( e \) and \( e' \), then form an even cycle \( C'' = P \cup P' \).

If \(|P''| \geq |P'| - 1\), the conditions (a) and (b) are automatically satisfied. Then any pair of edges \( e \in P \) and \( e' \in P' \), that are diametrically opposite on \( C'' \), will give \( \delta_{e'} = 1 \). The number of such pairs is equal to

\[
\min\{|P|, |P''|\}, \quad \text{if } |P| + |P'| \text{ is even}
\]

\[
0, \quad \text{if } |P| + |P'| \text{ is odd}
\]

If \(|P''| < |P'| - 1\), let \( p'_a \) be the length of \( P' \) from \( a \) to \( e' \), and let \( p'_b \) be the length of \( P' \) from \( b \) to \( e' \). The conditions (a) and (b) then translate to

\[
|P''| + p'_a \geq p'_b, \quad |P''| + p'_b \geq p'_a,
\]

which, by using \( p'_a + p'_b = |P'| - 1 \), yields

\[
|P'| - |P''| - 1 \leq 2p'_a \leq |P'| + |P''| - 1
\]

(and the same double inequality holds for \( p'_b \) as well). Since the diametrically opposite edges \( e \) and \( e' \) on \( C'' \) have to belong to the paths \( P \) and \( P' \), respectively, we get that the number of pairs \((e, e')\) with \( \delta_{e'} = 1 \) is equal to

\[
\min\{|P|, |P''|\}, \quad \text{if } |P'| + |P''| \text{ is even and } |P| + |P'| \text{ is even}
\]

\[
\min\{|P|, |P''| + 1\}, \quad \text{if } |P'| + |P''| \text{ is odd and } |P| + |P'| \text{ is even}
\]

\[
0, \quad \text{if } |P| + |P'| \text{ is odd}
\]

Combining the above results for all six choices of \( P, P' \in \{P_{q+1}, P_{r+1}, P_{s+1}\} \), we can get the total number of pairs \((e, e')\) with \( \delta_{e'} = 1 \) in this case, dependent upon the parity of the sums \( q + r, r + s \) and \( q + s \). The numbers of such pairs are given in Table 1.
Table 1: The results of case (iii) according to the parities of $q + r$, $r + s$ and $q + s$.

<table>
<thead>
<tr>
<th>$q + r$</th>
<th>$r + s$</th>
<th>$q + s$</th>
<th>The number of pairs $(e, e')$ with $\delta_{e'}^e = 1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>even</td>
<td>even</td>
<td>even</td>
<td>$4q + \begin{cases} r, &amp; \text{if } q \geq s - 1 \ q, &amp; \text{if } q &lt; s - 1 \end{cases}$</td>
</tr>
<tr>
<td>even</td>
<td>even</td>
<td>odd</td>
<td>$2q + \begin{cases} r, &amp; \text{if } q \geq s - 1 \ \min{r, q + 1}, &amp; \text{if } q &lt; s - 1 \end{cases}$</td>
</tr>
<tr>
<td>even</td>
<td>odd</td>
<td>even</td>
<td>$4q$</td>
</tr>
<tr>
<td>even</td>
<td>odd</td>
<td>odd</td>
<td>$2q$</td>
</tr>
<tr>
<td>odd</td>
<td>even</td>
<td>even</td>
<td>$2q + \begin{cases} r, &amp; \text{if } q \geq s - 1 \ q, &amp; \text{if } q &lt; s - 1 \end{cases}$</td>
</tr>
<tr>
<td>odd</td>
<td>even</td>
<td>odd</td>
<td>$\min{r, q + 1}$</td>
</tr>
<tr>
<td>odd</td>
<td>odd</td>
<td>even</td>
<td>$2q$</td>
</tr>
<tr>
<td>odd</td>
<td>odd</td>
<td>odd</td>
<td>$0$</td>
</tr>
</tbody>
</table>

3. Proof of Theorem 1: the maximum PI index among bicyclic graphs with constant number of vertices

According to (2), in order to prove Theorem 1, it is necessary to prove that $S^* \geq m + 4$, with equality if and only if $m$ is odd and $G \cong U_m$.

First, suppose that $G$ has disjoint cycles, then $S^* \geq m + 6$ by Lemma 4.

Next, suppose that the cycles of $G$ have edges in common, and let the union of their edge sets be isomorphic to $B_{q,r,s}$, with $q \leq r \leq s$ and with $a$ and $b$ as vertices of degree three in $B_{q,r,s}$.

If all of $q, r, s$ have the same parity, then from Lemma 5 and Eq. (10) we have that

$$S^* = t + \sum_{e \in B_{q,r,s}} \sum_{e' \in B_{q,r,s}} \delta_{e'}^e.$$ 

Since in this case all sums $q + r$, $r + s$ and $q + s$ are even, we further have from Lemma 6 and cases (i)-(iii) in Subsection 2.2.2. that

$$S^* = t + (q + r + s + (r - q) + (s - q)) + \left(4q + \begin{cases} r, & \text{if } q \geq s - 1 \\ q, & \text{if } q < s - 1 \end{cases}\right) \geq (t + q + r + s) + r + s + 4q \geq m + 6,$$

since $m = t + q + r + s$ and $q, r, s \geq 1$.

Next, suppose that not all of $q, r, s$ have the same parity. In that case, two among the sums $q + r$, $r + s$ and $q + s$ are odd, while only one of them is even. From Lemma 5 and Eq. (10) we have

$$S^* \geq 2t + \sum_{e \in B_{q,r,s}} \sum_{e' \in B_{q,r,s}} \delta_{e'}^e.$$
Further, from Lemma 6 and cases (i)-(iii) in Subsection 2.2.2, we have

\[
\sum_{e \in B_{q,r,s}} \sum_{e' \in B_{q,r,s}} \delta_{e,e'} \geq q + r + s + 2|\lfloor (r-q)/2 \rfloor|
\]

\[
+ \min \left( 2q, \begin{cases} \quad r, & \text{if } q \geq s - 1 \\ \min\{r, q+1\}, & \text{if } q < s - 1 \\ r, & \text{if } q \geq r - 1 \\ \min\{s, q+1\}, & \text{if } q < r - 1 \end{cases} \right)
\]

\[ \geq 3q + r + s. \]

Hence,

\[ S^* \geq 2t + 3q + r + s = m + t + 2q. \]

If \( q \geq 3 \), then \( S^* \geq m + 6. \)

Next, suppose that \( q = 2 \). Then from Lemma 6 and cases (i)-(iii) in Subsection 2.2.2, we get that:

(a) if \( r \) is even and \( s \) is odd, then

\[
S^* \geq 2t + (q + r + s + (r-q)) + 2(r-q)/2 + 2q = m + t + 2(r-q) + 4 \geq m + 4,
\]

since \( t \geq 0 \) and \( r \geq q \). The equality holds if and only if \( t = 0 \) and \( r = q = 2 \), i.e., for the graph \( U_m \).

(b) if \( r \) is odd and \( s \) is even, then

\[
S^* \geq 2t + (q + r + s + (s-q)) + 2(s-q)/2 + 2q = m + t + 2(s-q) + 4.
\]

Since an odd number \( r \) is placed between two even numbers \( q \) and \( s \), we have that \( s-q \geq 2 \), hence \( S^* \geq m + 8. \)

(c) if \( r \) is odd and \( s \) is odd, then \( r, s \geq 3 \) and

\[
S^* \geq 2t + (q + r + s) + 2((s-3)/2 + (r-3)/2) + 2r = m + t + s + 3r - 6.
\]

Since \( r, s \geq 3 \), we get \( S^* \geq m + 6. \)

Finally, suppose that \( q = 1 \). Then from Lemma 6 and cases (i)-(iii) in Subsection 2.2.2, we get that:

(d) if \( r \) is even and \( s \) is odd, then

\[
S^* \geq 2t + (q + r + s + (s-q)) + 2(s-q)/2 + 2q = m + t + 2s.
\]

Since an even number \( r \) is placed between odd numbers \( q \) and \( s \), we have that \( s \geq 3 \), hence \( S^* \geq m + 6. \)
(e) if $r$ is odd and $s$ is even, then
\[
S^* \geq 2t + (q + r + s + (r - q)) + 2(r - q)/2 + 2q
\]
\[
= m + t + 2r.
\]
Here $r = 1$ is impossible, as otherwise two parallel edges will exist between the common end vertices of $P_{q+1}$ and $P_{r+1}$. Hence, $r \geq 3$ and $S^* \geq m + 6$.

(f) if $r$ is even and $s$ is even, then
\[
S^* \geq 2t + (q + r + s) + 2((s - 2)/2 + (r - 2)/2)
\]
\[
+ \begin{cases} 
  r, & \text{if } 2 \geq r \\
  2, & \text{if } 2 < r
\end{cases}
\]
\[
\geq m + t + (s - 2) + (r - 2) + 4 = m + t + s + r \geq m + 4.
\]
The equality holds if and only if $t = 0$ and $s = r = 2$, i.e., for the unique graph $K_4 - e \cong U_5$.

Remark. It is evident from the above discussion that the second smallest feasible value for $S^*$ is $m + 6$ and that the case of equality $S^* = m + 6$ may be characterized, although it becomes cumbersome to enumerate the different graph types satisfying this equality.

4. Proof of Theorem 2: the minimum PI index among bicyclic graphs with constant number of vertices

According to (2), in order to prove Theorem 2, it is necessary to prove that $S^* \leq 3m$ for $m \equiv 0 \pmod{3}$, and $S^* \leq 3m - 2$ otherwise, with equality if and only if $G \in L_m$.

First, if $G$ has disjoint cycles, then $S^* \leq 3m - 6$ by Lemma 3.

Next, suppose that the cycles of $G$ have edges in common, and let the union of their edge sets be isomorphic to $B_{q,r,s}$, with $q \leq r \leq s$ and with $a$ and $b$ as vertices of degree three in $B_{q,r,s}$.

If all of $q, r, s$ have the same parity, then from Lemma 5 and Eq. (10) we have that
\[
S^* = t + \sum_{e \in B_{q,r,s}} \sum_{e' \in B_{q,r,s}} \delta_{e,e'}.
\]

Since in this case all sums $q + r$, $r + s$ and $q + s$ are even, we further have from Lemma 6 and cases (i)-(iii) in Subsection 2.2.2. that
\[
S^* = t + (q + r + s + (r - q) + (s - q)) + 2. 
\]
\[
+ \begin{cases} 
  4q + \{ r, & \text{if } q \geq s - 1 \\
  q, & \text{if } q < s - 1
\end{cases}
\]
\[
+ \begin{cases} 
  r, & \text{if } q \geq r - 1 \\
  q, & \text{if } q < r - 1
\end{cases}.
\]
If $q < r - 1$, then also $q < s - 1$ and (11) reduces to
\[
S^* = t + q + r + s + (r - q) + (s - q) + 4q + q + q = t + 5q + 2r + 2s.
\]
Since $r$ and $s$ are strictly greater than $q$ and have the same parity as $q$, we get $q \leq r - 2, s - 2$. Hence, $2q \leq r + s - 4$ and

$$S^* \leq t + 3q + 3r + 3s - 4 \leq 3m - 4,$$

since $m = t + q + r + s$.

If $q \geq s - 1$, then also $q \geq r - 1$ and (11) reduces to

$$S^* = t + q + r + s + (r - q) + (s - q) + 4q + r + r = t + 3q + 4r + 2s.$$

Since $r$ and $s$ are at most $q + 1$ and have the same parity as $q$, we get $q = r = s$.

Hence

$$S^* = t + 3q + 3r + 3s \leq 3m,$$

with equality if and only if $t = 0$ and $G \cong L_m$.

Otherwise, we have $r - 1 \leq q < s - 1$. The equation (11) reduces to

$$S^* = t + q + r + s + (r - q) + (s - q) + 4q + q + r = t + 4q + 3r + 2s.$$

Since $s$ is strictly greater than $q$ and has the same parity as $q$, we get $q \leq s - 2$.

Hence

$$S^* \leq t + 3q + 3r + 3s - 2 \leq 3m - 2,$$

with equality if and only if $t = 0$, $r = q$, $s = q + 2$ and $G \cong L_m$.

Next, suppose that not all of $q, r, s$ have the same parity. In that case, two among the sums $q + r$, $r + s$ and $q + s$ are odd, while only one of them is even.

From Lemma 5 and Eq. (10) we have

$$S^* \leq 3t + \sum_{e \in B_{q,r,s}} \sum_{e' \in B_{q,r,s}} \delta_{e'}^e.$$

Further, from Lemma 6 and cases (i)-(iii) in Subsection 2.2.2. we have

$$\sum_{e \in B_{p,q,r,s}} \sum_{e' \in B_{p,q,r,s}} \delta_{e'}^e \leq$$

$$(q + r + s + (s - q)) + 2(\lfloor (r - q)/2 \rfloor + \lfloor (s - q)/2 \rfloor)$$

$$+ \begin{cases} r, & \text{if } q \geq s - 1 \\ \min\{r, q + 1\}, & \text{if } q < s - 1 \end{cases} + \begin{cases} r, & \text{if } q \geq r - 1 \\ \min\{s, q + 1\}, & \text{if } q < r - 1 \end{cases}.$$

If $q < r - 1$, then also $q < s - 1$ and (12) reduces to

$$\sum_{e \in B_{q,r,s}} \sum_{e' \in B_{q,r,s}} \delta_{e'}^e \leq$$

$$r + 2s + 2(\lfloor (r - q)/2 \rfloor + \lfloor (s - q)/2 \rfloor)$$

$$+ \min\{r, q + 1\} + \min\{s, q + 1\}$$

$$\leq r + 2s + (r - q) + (s - q) + 2(q + 1)$$

$$= 2r + 3s + 2.$$

From $1 \leq q$ and $3 \leq r$ (as $q < r - 1$), we get that $2r + 3s + 2 \leq 3q + 3r + 3s - 4$, hence $S^* \leq 3t + 3q + 3r + 3s - 3 = 3m - 4$. 

12
If \( q \geq s - 1 \), then also \( q \geq r - 1 \) and (12) reduces to

\[
\sum_{e \in B_{q,r,s}} \sum_{e' \in B_{q,r,s}} \delta_{ee}' \leq r + 2s + 2 \left( \left\lfloor \frac{r-q}{2} \right\rfloor + \left\lfloor \frac{s-q}{2} \right\rfloor \right) + r + r = 3r + 2s.
\]

From \( 1 \leq q \) and \( 2 \leq s \) (as not all of \( q,r,s \) have the same parity), we get that \( 3r + 2s \leq 3q + 3r + 3s - 5 \), hence \( S^* \leq 3t + 3q + 3r + 3s - 5 = 3m - 5 \).

Otherwise, we have \( r - 1 \leq q < s - 1 \) and (12) reduces to

\[
\sum_{e \in B_{q,r,s}} \sum_{e' \in B_{q,r,s}} \delta_{ee}' \leq r + 2s + 2 \left( \left\lfloor \frac{r-q}{2} \right\rfloor + \left\lfloor \frac{s-q}{2} \right\rfloor \right) + \min\{r, q+1\} + r = -q + 3r + 3s.
\]

From \( 1 \leq q \) we get that \( -q + 3r + 3s \leq 3q + 3r + 3s - 4 \), hence \( S^* \leq 3t + 3q + 3r + 3s - 4 = 3m - 4 \).

**Remark.** It is evident from the above discussion that the third largest feasible value for \( S^* \) is \( 3m - 4 \) and that the case of equality \( S^* = 3m - 4 \) may be characterized, although it becomes cumbersome to enumerate the different graph types satisfying this equality.

**Acknowledgement.** The authors are indebted to an anonymous referee for carefully reading the proofs and spotting a few minor notational mistakes in the initial version of the manuscript.


