

New upper bounds for the forgotten index among bicyclic graphs

A. Jahanbani^{a*}, L. Shahbazi^a, S.M. Sheikholeslami^a,
R. Rasi^a, and J. Rodríguez^b

^a*Department of Mathematics, Azarbaijan Shahid Madani University
Tabriz, Iran*

^b*Departamento de Matemáticas, Facultad de Ciencias Básicas, Universidad de
Antofagasta, Av Angamos 601, Antofagasta, Chile.*

Abstract

The forgotten topological index of a graph G , denoted by $F(G)$, is defined as the sum of weights $d(u)^2 + d(v)^2$ over all edges uv of G , where $d(u)$ denotes the degree of a vertex u . In this paper, we give sharp upper bounds of the F-index (forgotten topological index) over bicyclic graphs, in terms of the order and maximum degree.

Keywords: Forgotten index, Bicyclic graph, Molecular graph, Maximum degree

AMS subject classification: 05C50, 92E10

1 Introduction

A topological index is a numeric quantity associated with a molecular graph that remains invariant under graph isomorphism and encodes at least one physical or chemical property of the underlying organic molecule. Topological indices play an important role in predicting the physical as well as the chemical properties (boiling point, volatility, stability, solubility, connectivity, chirality and melting point) of chemical compounds. For more information we refer to [12, 13] and the references cited therein.

Let G be a simple graph with vertex set $V = V(G)$ and edge set $E = E(G)$. The integers $n = n(G) = |V(G)|$ and $m = m(G) = |E(G)|$ are the order and the size of the graph G , respectively. If $m = n + 1$ then we say that G is a bicyclic graph. The open neighborhood of vertex v is defined as $N(v) = N_G(v) = \{u \in V(G) : uv \in E(G)\}$ and the degree of v is $d_G(v) = d_v = |N(v)|$. The maximum degree of a graph G is denoted by $\Delta = \Delta(G)$.

*Corresponding author.

E-mail addresses: Akbar.jahanbani92@gmail.com (A. Jahanbani),
s.m.sheikholeslami@azaruniv.ac.ir (S.M. Sheikholeslami), l.shahbazi@azaruniv.ac.ir (L. Shahbazi), r.rasi@azaruniv.edu (R. Rasi), jonnathan.rodriguez@uantof.cl (J. Rodríguez)

Our main objective in this paper is to investigate the forgotten index, denoted by $F(G)$ for a graph G and defined as

$$F = F(G) = \sum_{uv \in E} [d(u)^2 + d(v)^2] = \sum_{v \in V} d(v)^3.$$

This topological index was named and first studied by Furtula and Gutman [6] in 2015, but it first appeared in 1972 [8] within the study of structure-dependency of the total π -electron energy. For recent results in the F-index of graphs we refer to [1, 4, 5, 7, 9–11]. In this paper, we established sharp upper bounds for the F-index among bicyclic graphs, in terms of the order and the maximum degree.

2 Upper bounds on the Forgotten topological index of bicyclic graphs

In this section, we establish new upper bounds for the forgotten topological index of bicyclic graphs. Now we present some known results that will be needed in this section.

If n is a positive integer, then an integer partition of n is a non-increasing sequence of positive integers $y = (x_1, x_2, \dots, x_t)$, such that $n = \sum_{i=1}^t x_i$. If $\Delta \geq x_1 \geq x_2 \geq \dots \geq x_t \geq 1$, then (x_1, x_2, \dots, x_t) is called a Δ -partition or an integer partition of n on $N_\Delta = \{1, 2, \dots, \Delta\}$.

A Δ -partition $y = (y_1, y_2, \dots, y_t)$ of n is called an integer Δ -dominant sequence if the number Δ in this partition is as large as possible. In other words, if $n = t\Delta$, then $y = (\Delta, \dots, \Delta)$ is the integer Δ -dominant sequence and if $n = t\Delta + b$ where $0 < b < \Delta$ then $y = (\Delta, \dots, \Delta, b)$ is the integer Δ -partition.

Let B be a bicyclic graph of order n and maximum degree Δ . For each $i \in \{1, 2, \dots, \Delta\}$, let n_i denote the number of vertices of degree i . Then

$$n_1 + n_2 + \dots + n_\Delta = n \tag{1}$$

and

$$n_1 + 2n_2 + \dots + \Delta n_\Delta = 2m = 2n. \tag{2}$$

Subtracting (1) from (2), yields

$$n_2 + 2n_3 + \dots + (\Delta - 1)n_\Delta = n. \tag{3}$$

By (3), we obtain the $(\Delta - 1)$ -partition of n as follows:

$$(\underbrace{\Delta - 1, \dots, \Delta - 1}_{n_\Delta}, \dots, \underbrace{2, \dots, 2}_{n_3}, \underbrace{1, \dots, 1}_{n_2}). \quad (4)$$

Next result is an immediate consequence of the above discussion.

Corollary 1. *For any bicyclic graph B of order n with maximum degree Δ , the F -index $F(B) = \sum_{v \in V} d_v^3$ is maximum if and only if the $(\Delta - 1)$ -partition (4) is a $(\Delta - 1)$ -dominant sequence of n .*

Remark 2. *In other words, with regard to the $(\Delta - 1)$ -dominant sequence of n , n_Δ (number of vertices with degree $\Delta - 1$) must be maximum. In this case, sequence $(n_1, n_2, \dots, n_\Delta)$ is called a major sequence for B .*

Theorem 3. *Let B be a bicyclic graph of order n and maximum degree Δ with $n \equiv 0 \pmod{\Delta - 1}$. Then*

$$F(B) \leq (\Delta^2 + \Delta + 2)n + 26$$

Proof. Without loss of generality, assume that $n = (\Delta - 1)k$.

By equality in (4), we have

$$n_\Delta = \frac{n + 2 - (n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1})}{\Delta - 1} = k - r$$

where

$$r = \frac{n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} - 2}{\Delta - 1}.$$

then $-1 \leq r \leq k - 1$ and $1 \leq n_\Delta \leq k$.

Thus, consider the following cases.

Case 0. $r = -1$.

Then, clearly $n_\Delta = k + 1$. It follows that

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} + (\Delta - 1)(k + 1) = (\Delta - 1)k + 2$$

and so

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = -(\Delta - 1) + 2$$

that it is not possible. so $r = 0$, $\Delta > 3$.

Case 1. $r = 0$.

Thus, $n_\Delta = k$, $n_3 = 1$, $n_2 = \dots = n_{\Delta-1} = 0$. Since $n_1 + n_2 + \dots + n_\Delta = n$, we conclude that $n_1 = (\Delta - 2)k - 1$. By Corollary 1, we obtain

$$(n_1, n_2, n_3, \dots, n_{\Delta-1}, n_\Delta) = ((\Delta - 2)k - 1, 0, 1, 0, \dots, 0, k)$$

which is the optimal solution and so $F(B)$ is maximum. Therefore,

$$\begin{aligned} F(B) &\leq F_{\max}(B_{n,\Delta}) = n_1 + 2^3 n_2 + \dots + (\Delta - 1)^3 n_{\Delta-1} + \Delta^3 n_\Delta \\ &= (\Delta - 2)k - 1 + 3^3 + \Delta^3(k) \\ &= (\Delta^3 + \Delta - 2)k + 26 \\ &= (\Delta^2 + \Delta + 2)(\Delta - 1)k + 26 \\ &= (\Delta^2 + \Delta + 2)n + 26. \end{aligned}$$

Case 2. $r = 1$.

Since $n_\Delta = k - 1$, it follows from (4) that

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 1) + 2 = (\Delta - 2) + 3.$$

First let $\Delta > 4$, so, $n_4 = 1$, $n_{\Delta-1} = 1$, $n_2 = \dots = n_{\Delta-2} = 0$. Since $n_1 + n_2 + \dots + n_\Delta = n$, we conclude that $n_1 = (\Delta - 2)k - 1$. By Corollary 1,

$$(n_1, n_2, n_3, n_4, \dots, n_{\Delta-1}, n_\Delta) = ((\Delta - 2)k - 1, 0, 0, 1, 0, \dots, 0, k - 1)$$

which is the optimal solution and so $F(B)$ is maximum. Therefore,

$$\begin{aligned} F(B) &\leq F_{\max}(B_{n,\Delta}) = n_1 + 2^3 n_2 + \dots + (\Delta - 1)^3 n_{\Delta-1} + \Delta^3 n_\Delta \\ &= (\Delta - 2)k - 1 + 4^3 + (\Delta - 1)^3 + \Delta^3(k - 1) \\ &= (\Delta^3 + \Delta - 2)k + 63 - 3\Delta^2 + 3\Delta - 1 \\ &= (\Delta^3 + \Delta - 2)k - 3\Delta^2 + 3\Delta + 62 \\ &= (\Delta^2 + \Delta + 2)(\Delta - 1)k - 3\Delta(\Delta - 1) + 62 \\ &\leq (\Delta^2 + \Delta + 2)n - 15(\Delta - 1) + 62 \\ &= (\Delta^2 + \Delta + 2)n - 15\Delta + 77 \\ &\leq (\Delta^2 + \Delta + 2)n + 2 \\ &< (\Delta^2 + \Delta + 2)n + 26. \end{aligned}$$

Now, if let $\Delta = 4$, by Corollary 1

$$(n_1, n_2, n_3, n_4) = (2k - 2, 1, 2, k - 1)$$

which is the optimal solution. Therefore,

$$\begin{aligned}
F(B) &\leq F_{\max}(B_{n,\Delta}) = n_1 + 2^3 n_2 + 3^3 n_3 + 4^3 n_4 \\
&= (2k - 2) + 8 + 3^3(2) + 4^3(k - 1) \\
&= (4^3 + 4 - 2)k - 4 \\
&= (\Delta^3 + \Delta - 2)k - 4 \\
&= (\Delta^2 + \Delta + 2)(\Delta - 1)k - 4 \\
&= (\Delta^2 + \Delta + 2)n - 4 \\
&< (\Delta^2 + \Delta + 2)n + 26.
\end{aligned}$$

Also, if $\Delta = 3$, by Corollary 1

$$(n_1, n_2, n_3) = (k - 3, 4, k - 1)$$

which is the optimal solution. Thus,

$$\begin{aligned}
F(B) &\leq F_{\max}(B_{n,\Delta}) = n_1 + 2^3 n_2 + 3^3 n_3 \\
&= (k - 3) + 8(4) + 3^3(k - 1) \\
&= (3^3 + 3 - 2)k + 2 \\
&= (\Delta^3 + \Delta - 2)k + 2 \\
&= (\Delta^2 + \Delta + 2)(\Delta - 1)k + 2 \\
&= (\Delta^2 + \Delta + 2)n + 2 \\
&< (\Delta^2 + \Delta + 2)n + 26.
\end{aligned}$$

Case 3. $2 \leq r < \Delta - 3$.

As above,

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 1)r + 2 = (\Delta - 2)r + r + 2.$$

since $r + 2 < \Delta - 1$, it follows from Corollary 1 that

$$(n_1, n_2, \dots, n_{r+3}, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k - 1, 0, \dots, 1, \dots, 0, r, k - r)$$

which is the optimal solution. Thus

$$F(B) \leq F_{\max}(B_{n,\Delta}) = n_1 + 2^3 n_2 + \dots + (\Delta - 1)^3 n_{\Delta-1} + \Delta^3 n_{\Delta}$$

$$\begin{aligned}
&= (\Delta - 2)k - 1 + (r + 3)^3 + (\Delta - 1)^3 r + \Delta^3(k - r) \\
&= (\Delta^3 + \Delta - 2)k - 1 + (r + 3)^3 - 3\Delta^2 r + 3\Delta r - r \\
&= (\Delta^2 + \Delta + 2)n + (r + 3)^3 - 3\Delta^2 r + 3\Delta r - r - 1 \\
&= (\Delta^2 + \Delta + 2)n + (r + 3)^3 + r(-3\Delta^2 + 3\Delta - 1) - 1 \\
&< (\Delta^2 + \Delta + 2)n + \Delta^3 + (\Delta - 3)(-3\Delta^2 + 3\Delta - 1) - 1 \\
&= (\Delta^2 + \Delta + 2)n - 2\Delta^3 + 12\Delta^2 - 10\Delta + 2 \\
&= (\Delta^2 + \Delta + 2)n - \Delta^2(2\Delta - 12) - 10\Delta + 2 \\
&< (\Delta^2 + \Delta + 2)n - 25(2\Delta - 12) - 50 + 2 \\
&= (\Delta^2 + \Delta + 2)n - 50\Delta + 252 \\
&< (\Delta^2 + \Delta + 2)n + 2 \\
&< (\Delta^2 + \Delta + 2)n + 26.
\end{aligned}$$

Because $5 < \Delta$.

Case 4. $\Delta - 3 \leq r \leq k - 1$. Then

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)r + r + 2.$$

Thereby, there are non-negative integers t, s such that $r + 2 = t(\Delta - 2) + s$ with $0 \leq s < \Delta - 2$. Hence

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)(r + t) + s.$$

If $0 < s < \Delta - 2$, then

$$(n_1, n_2, \dots, n_s, n_{s+1}, n_{s+2}, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k - (t + 1), 0, \dots, 0, 1, 0, \dots, 0, 0, t + r, k - r)$$

which is optimal solution and since $s < \Delta - 2$ and $-r \leq 3 - \Delta$ and $\Delta > 5$, we obtain

$$\begin{aligned}
F(B) &\leq n_1 + 2^3 n_2 + \dots + (\Delta - 1)^3 n_{\Delta-1} + \Delta^3 n_{\Delta} \\
&= (\Delta - 2)k - (t + 1) + (s + 1)^3 + (\Delta - 1)^3(t + r) + \Delta^3(k - r) \\
&= (\Delta^3 + \Delta - 2)k - t - 1 + (s + 1)^3 + \Delta^3 t - 3\Delta^2 t + 3\Delta t - t - 3\Delta^2 r + 3\Delta r - r \\
&= (\Delta^3 + \Delta - 2)k + (s + 1)^3 - 1 - t(-\Delta^3 + 3\Delta^2 - 3\Delta + 2) - r(3\Delta^2 + 3\Delta + 1) \\
&< (\Delta^3 + \Delta - 2)k + (\Delta - 1)^3 - 1 - 1(-\Delta^3 + 3\Delta^2 - 3\Delta + 2) + (3 - \Delta)(3\Delta^2 + 3\Delta + 1) \\
&= (\Delta^2 + \Delta + 2)n - \Delta^3 + 6\Delta^2 - 4\Delta - 1
\end{aligned}$$

$$\begin{aligned}
&= (\Delta^2 + \Delta + 2)n - \Delta^2(\Delta - 6) - 4\Delta - 1 \\
&< (\Delta^2 + \Delta + 2)n - 25(\Delta - 6) - 21 \\
&= (\Delta^2 + \Delta + 2)n - 25\Delta + 129 \\
&< (\Delta^2 + \Delta + 2)n + 4 \\
&< (\Delta^2 + \Delta + 2)n + 26.
\end{aligned}$$

If $s = 0$, then the optimal solution is

$$(n_1, n_2, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k - t, 0, \dots, 0, r + t, k - r).$$

Since $-r < (4 - \Delta)$, $\Delta > 3$, we conclude that

$$\begin{aligned}
F(B) &\leq n_1 + 2^3 n_2 + \dots + (\Delta - 1)^3 n_{\Delta-1} + \Delta^3 n_{\Delta} \\
&= (\Delta - 2)k - t + \Delta^3 t - 3\Delta^2 t + 3\Delta t - t - 3\Delta^2 r + 3\Delta r - r \\
&= (\Delta^3 + \Delta - 2)k - t(-\Delta^3 + 3\Delta^2 - 3\Delta + 2) - r(3\Delta^2 - 3\Delta + 1) \\
&< (\Delta^3 + \Delta - 2)k - 1(-\Delta^3 + 3\Delta^2 - 3\Delta + 2) + (4 - \Delta)(3\Delta^2 - 3\Delta + 1) \\
&= (\Delta^2 + \Delta + 2)n - 2\Delta^3 + 12\Delta^2 - 10\Delta + 2 \\
&= (\Delta^2 + \Delta + 2)n - 2\Delta^2(\Delta - 6) - 10\Delta + 2 \\
&< (\Delta^2 + \Delta + 2)n - 50(\Delta - 6) - 48 \\
&= (\Delta^2 + \Delta + 2)n - 50\Delta + 252 \\
&< (\Delta^2 + \Delta + 2)n - 2 \\
&< (\Delta^2 + \Delta + 2)n + 26.
\end{aligned}$$

□

Theorem 4. *Let B be a bicyclic graph of order n and maximum degree Δ with $n \equiv 1 \pmod{\Delta - 1}$. Then*

$$F(B) \leq (\Delta^2 + \Delta + 2)n - (\Delta^2 + \Delta - 6).$$

Proof. Let $n = (\Delta - 1)k + 1$. Set

$$r = \frac{n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} - 3}{\Delta - 1}.$$

By equality in (4), we have

$$n_{\Delta} = k - \left(\frac{n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} - 3}{\Delta - 1} \right) = k - r.$$

Then clearly $-1 \leq r \leq k-1$ and $1 \leq n_\Delta \leq k$. We consider the following cases:

Case 0. $r = -1$.

Then clearly $n_\Delta = k+1$. It follow that

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} + (\Delta - 1)(k+1) = (\Delta - 1)k + 3$$

and so

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = -(\Delta - 1) + 3$$

that it is not possible. so $r = 0$, $\Delta > 3$.

Case 1. $r = 0$.

Since

$$r = \frac{n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} - 3}{\Delta - 1} = 0,$$

it follows that $n_4 = 1$, $n_2 = \dots = n_{\Delta-1} = 0$ and $n_\Delta = k$. From (2), we have $n_1 = (\Delta - 2)k$.

Now, by Corollary 1, we have

$$(n_1, n_2, n_3, n_4, \dots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta - 2)k, 0, 0, 1, 0, \dots, 0, k)$$

which is the optimal solution. Thus

$$\begin{aligned} F(B) &\leq F_{\max}(B_{n,\Delta}) = n_1 + 2^3 n_2 + \dots + (\Delta - 1)^3 n_{\Delta-1} + \Delta^3 n_\Delta \\ &= (\Delta - 2)k + 8 + \Delta^3(k) \\ &= (\Delta^3 + \Delta - 2)k + 8 \\ &= (\Delta^2 + \Delta + 2)(\Delta - 1)k + 8 \\ &= (\Delta^2 + \Delta + 2)(n - 1) + 8 \\ &= (\Delta^2 + \Delta + 2)n - (\Delta^2 + \Delta - 6). \end{aligned}$$

Case 2. $r = 1$

Since $n_\Delta = k-1$, it follows from (4) that

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 1) = (\Delta - 2) + 4.$$

First let $\Delta > 5$. By Corollary 1,

$$(n_1, n_2, n_3, n_4, \dots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta - 2)k - 1, 0, 2, 0, \dots, 0, 1, k - 1)$$

which is the optimal solution. Thus

$$\begin{aligned}
F(B) &\leq F_{\max}(B_{n,\Delta}) = n_1 + 2^3 n_2 + \dots + (\Delta - 1)^3 n_{\Delta-1} + \Delta^3 n_{\Delta} \\
&= (\Delta - 2)k + 53 + (\Delta + 1)^3 + \Delta^3(k - 1) \\
&= (\Delta^3 + \Delta - 2)k + 52 - 3\Delta^2 + 3\Delta \\
&= (\Delta^2 + \Delta + 2)(n - 1) + 52 - 3\Delta^2 + 3\Delta \\
&= (\Delta^2 + \Delta + 2)n - 4\Delta^2 + 2\Delta + 50 \\
&= (\Delta^2 + \Delta + 2)n - 4(\Delta^2 + \Delta - 6) + 6\Delta + 26 \\
&< (\Delta^2 + \Delta + 2)n - (\Delta^2 + \Delta - 6).
\end{aligned}$$

Now, if let $\Delta = 5$, by Corollary 1,

$$(n_1, n_2, n_3, n_4, n_5) = (3k - 1, 0, 2, 1, k - 1)$$

which is the optimal solution. Thus

$$\begin{aligned}
F(B) &\leq F_{\max}(B_{n,\Delta}) = n_1 + 2^3 n_2 + 3^3 n_3 + 4^3 n_4 + 5^3 n_5 \\
&= 3k - 1 + 54 + 64 + 5^3(k - 1) \\
&= (5^3 + 5 - 2)k - 8 \\
&= (\Delta^3 + \Delta - 2)k - 8 \\
&= (\Delta^2 + \Delta + 2)(\Delta - 1)k - 8 \\
&= (\Delta^2 + \Delta + 2)(n - 1) - 8 \\
&= (\Delta^2 + \Delta + 2)n - (\Delta^2 + \Delta + 10) \\
&= (\Delta^2 + \Delta + 2)n - (\Delta^2 + \Delta - 6) - 16 \\
&< (\Delta^2 + \Delta + 2)n - (\Delta^2 + \Delta - 6).
\end{aligned}$$

Also, if let $\Delta = 4$. By Corollary 1,

$$(n_1, n_2, n_3, n_4) = (2k - 2, 2, 2, k - 1)$$

which is the optimal solution. Thus

$$\begin{aligned}
F(B) &\leq F_{\max}(B_{n,\Delta}) = n_1 + 2^3 n_2 + 3^3 n_3 + 4^3 n_4 \\
&= 2k - 2 + 16 + 54 + 4^3(k - 1) \\
&= (4^3 + 4 - 2)k + 4
\end{aligned}$$

$$\begin{aligned}
&= (\Delta^3 + \Delta - 2)(n - 1) + 4 \\
&= (\Delta^2 + \Delta + 2)n - (\Delta^2 + \Delta - 2) \\
&= (\Delta^2 + \Delta + 2)n - (\Delta^2 + \Delta - 6) - 4 \\
&< (\Delta^2 + \Delta + 2)n - (\Delta^2 + \Delta - 6).
\end{aligned}$$

Case 3. $2 \leq r < \Delta - 4$

Since $2 \leq r < \Delta - 4$, thus $\Delta > 6$. In this case:

$$\text{Hypothesis : } \begin{cases} n = (\Delta - 1)k + 1 \\ 2 \leq r = \frac{n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} - 3}{\Delta - 1} < \Delta - 4 \\ n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)r + (r + 3) \\ r + 1 \leq \Delta - 4 \\ n_{\Delta} = k - r \\ n_{\Delta-1} = r \\ n_{r+4} = 1 \\ n_1 = (\Delta - 2)k \end{cases}$$

and from Corollary 1 we obtain

$$(n_1, n_2, \dots, n_{r+3}, n_{r+4}, n_{r+5}, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k, 0, \dots, 0, 1, 0, \dots, 0, r, k - r)$$

which which is the optimal optimization. Then

$$\begin{aligned}
F(U) &\leq F_{\max}(U_{n,\Delta}) = n_1 + 2^3 n_2 + \dots + (\Delta - 1)^3 n_{\Delta-1} + \Delta^3 n_{\Delta} \\
&= (\Delta - 2)k + (r + 4)^3 + (\Delta - 1)^3 r + \Delta^3 (k - r) \\
&< (\Delta^3 + \Delta - 2)k + \Delta^3 + r(-3\Delta^2 + 3\Delta - 1) \\
&= (\Delta^2 + \Delta + 2)(n - 1) + (r + 2)^3 + r(-3\Delta^2 + 3\Delta - 1) \\
&< (\Delta^2 + \Delta + 2)n - \Delta^2 - \Delta - 2 + (\Delta - 4)(-3\Delta^2 + 3\Delta - 1) \\
&= (\Delta^2 + \Delta + 2)n - 2\Delta^3 + 14\Delta^2 - 14\Delta + 4 \\
&= (\Delta^2 + \Delta + 2)n - (2\Delta - 16)(\Delta^2 + \Delta - 6) - 42\Delta + 100 \\
&< (\Delta^2 + \Delta + 2)n - (\Delta^2 + \Delta - 6).
\end{aligned}$$

Since $\Delta > 6$.

Case 4. $\Delta - 4 \leq rk - 4$. Then, there are non-negative integers t, s such that $r + 3 = t(\Delta - 2) + s$, $t \geq 1$ and $0 \leq s < \Delta - 2$. By substituting in (4), we have

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)(r + t) + s.$$

$$Hypothesis : \begin{cases} n = (\Delta - 2)k - (t + 1) \\ \Delta - 4 \leq r = \frac{n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} - 3}{\Delta - 1} \leq k - 1 \\ n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)(r + t) + s \\ s + 1 \leq \Delta - 2 \\ n_{\Delta} = k - r \\ n_{\Delta-1} = r + t \\ n_{s+1} = 1 \\ n_1 = (\Delta - 2)k - (t + 1) \end{cases}$$

First let $0 < s$. From Corollary 1, we have

$$(n_1, n_2, \dots, n_s, n_{s+1}, n_{s+2}, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k - (t + 1), 0, \dots, 0, 1, 0, \dots, 0, 0, r + t, k - r)$$

which is the optimal solution. Thus

$$\begin{aligned} F(B) &\leq F_{\max}(B_{n,\Delta}) = n_1 + 2^3 n_2 + \dots + (\Delta - 1)^3 n_{\Delta-1} + \Delta^3 n_{\Delta} \\ &= (\Delta - 2)k - (t + 1) + (s + 1)^3 + (\Delta - 1)^3(t + r) + \Delta^3(k - r) \\ &= (\Delta^3 + \Delta - 2)k - 1 + (s + 1)^3 - t(\Delta^3 + 3\Delta^2 - 3\Delta + 2) - r(3\Delta^2 - 3\Delta + 1) \\ &< (\Delta^3 + \Delta - 2)k - 1 + (\Delta - 1)^3 - 1(\Delta^3 + 3\Delta^2 - 3\Delta + 2) + (4 - \Delta)(3\Delta^2 - 3\Delta + 1) \\ &= (\Delta^2 + \Delta + 2)n - \Delta^3 + 8\Delta^2 - 8\Delta - 2 \\ &= (\Delta^2 + \Delta + 2)n + (\Delta - 9)(-\Delta^2 - \Delta + 6) - 23\Delta + 52 \\ &< (\Delta^2 + \Delta + 2)n + (\Delta^2 + \Delta - 6). \end{aligned}$$

Now let $s = 0$, then the optimal solution is

$$(n_1, n_2, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k - t + 1, 0, \dots, 0, r + t, k - r).$$

where we have that

$$Hypothesis : \begin{cases} n = (\Delta - 1)k + 1 \\ \Delta - 4 \leq r = \frac{n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} - 3}{\Delta - 1} < k - 1 \\ n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)(r + t) \\ n_{\Delta} = k - r \\ n_{\Delta-1} = r + t \\ n_2 = n_3 = \dots = n_{\Delta-2} = 0 \\ n_1 = (\Delta - 2)k - t + 1. \end{cases}$$

Therefore

$$\begin{aligned} F(B) &\leq F_{\max}(B_{n,\Delta}) = n_1 + 2^3 n_2 + \dots + (\Delta - 1)^3 n_{\Delta-1} + \Delta^3 n_{\Delta} \\ &= (\Delta - 2)k - t + 1 + (\Delta - 1)^3(t + r) + \Delta^3(k - r) \\ &= (\Delta^3 + \Delta - 2)k - t(\Delta^3 + 3\Delta^2 - 3\Delta + 2) + 1 - r(3\Delta^2 - 3\Delta + 1) \end{aligned}$$

$$\begin{aligned}
&< (\Delta^3 + \Delta - 2)k - 1(\Delta^3 + 3\Delta^2 - 3\Delta + 2) + 1 + (4 - \Delta)(3\Delta^2 - 3\Delta + 1) \\
&= (\Delta^2 + \Delta + 2)n - 2\Delta^3 + 11\Delta^2 - 11\Delta + 1 \\
&= (\Delta^2 + \Delta + 2)n + (2\Delta - 13)(-\Delta^2 - \Delta + 6) + 36\Delta + 79 \\
&< (\Delta^2 + \Delta + 2)n - (\Delta^2 + \Delta - 6).
\end{aligned}$$

□

Theorem 5. Let B be a bicyclic graph of order n and maximum degree Δ with $n \equiv p \pmod{\Delta - 1}$ where $2 \leq p < \Delta - 3$. Then

$$F(B) \leq (\Delta^2 + \Delta + 2) - p(\Delta^2 + \Delta + 2) + p^3 + 9p^2 + 28p + 26.$$

Proof. Let $n = (\Delta - 1)k + p$. Suppose that

$$r = \frac{n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} - p - 2}{\Delta - 1}.$$

By equality in (4), we have

$$n_{\Delta} = k - \left(\frac{n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} - p - 2}{\Delta - 1} \right) = k - r.$$

Then clearly $-1 \leq r \leq k - 1$ and $1 \leq n_{\Delta} \leq k$. We consider the following cases.

Case 0. $r = -1$.

Then clearly $n_{\Delta} = k + 1$. It follow that

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} + (\Delta - 1)(k + 1) = (\Delta - 1)k + p + 2$$

and so

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = -(\Delta - 1) + (p + 2)$$

that it is not possible. So $r = 0$, $\Delta - 1 \geq p + 2$ implies that $\Delta \geq p + 3$. We consider $2 \leq p \leq \Delta - 3$.

Case 1. $r = 0$.

Then $n_{\Delta} = k$ and we by (4) we have

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 1)k + p + 2 - (\Delta - 1)k = p + 2.$$

it follows from Corollary (6) that

$$(n_1, n_2, \dots, n_{p+3}, \dots, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k + p - 1, 0, \dots, 0, 1, 0, \dots, 0, k)$$

which is the optimal solution and so

$$\begin{aligned}
F(B) &\leq F_{\max}(B_{n,\Delta}) = n_1 + 2^3 n_2 + \dots + \Delta^3 n_\Delta \\
&= (\Delta - 2)k + p - 1 + (p + 3)^3 + \Delta^3(k) \\
&= (\Delta^3 + \Delta - 2)k + p^3 + 9p^2 + 28p + 26 \\
&= (\Delta^2 + \Delta + 2)n - p(\Delta^2 + \Delta + 2) + p^3 + 9p^2 + 28p + 26.
\end{aligned}$$

Case 2. $r = 1$.

Then $n_\Delta = k - 1$ and by (4) we have

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 1) + p + 2 = (\Delta - 2) + (p + 3).$$

Since $5 \leq p + 3 < \Delta$, we consider three subcases:

Subcase 2.1 $p + 3 = \Delta - 1$.

Then

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = 2(\Delta - 2) + 1.$$

Therefore

$$(n_1, n_2, \dots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta - 2)k + p - 2, 1, 0, \dots, 0, 2, k - 1)$$

which is the optimal solution and $p = \Delta - 2$ we have

$$\begin{aligned}
F(B) &\leq F_{\max}(B_{n,\Delta}) = n_1 + 2^3 n_2 + \dots + \Delta^3 n_\Delta \\
&= (\Delta - 2)k + p - 2 + 8 + 2(\Delta - 1)^3 + \Delta^3(k - 1) \\
&= (\Delta^3 + \Delta - 2)k + p + \Delta^3 - 6\Delta^2 + 6\Delta + 4 \\
&= (\Delta^2 + \Delta + 2)(n - p) + p(\Delta^2 - 4\Delta - 2) + p + \Delta^3 - 6\Delta^2 + 6\Delta + 4 \\
&= (\Delta^2 + \Delta + 2)(n - p) + p(\Delta^2 - 4\Delta - 2) + p + (\Delta - 2)(\Delta^2 - 4\Delta - 2) \\
&= (\Delta^2 + \Delta + 2)(n - p) + p(\Delta^2 - 4\Delta - 2) + p + (p + 2)(\Delta^2 - 4\Delta - 2) \\
&= (\Delta^2 + \Delta + 2)(n - p) + p(\Delta^2 - 4\Delta - 2) + 2\Delta^2 - 8\Delta - 4 \\
&= (\Delta^2 + \Delta + 2)n - p(5\Delta + 3) + 2\Delta^2 - 8\Delta - 4 \\
&< (\Delta^2 + \Delta + 2)n - p(\Delta^2 + \Delta + 2) + p^3 + 9p^2 + 28p + 26,
\end{aligned}$$

since $-p(5\Delta + 3) + 2\Delta^2 - 8\Delta - 4 < p^3 + 9p^2 + 28p + 26$.

Subcase 2.2 $p + 3 = \Delta - 2$.

Then $n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = 2(\Delta - 2)$. Therefore

$$(n_1, n_2, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k + p - 1, 0, \dots, 0, 2, k - 1)$$

which is the optimal solution and $p = \Delta - 3$ we have

$$\begin{aligned} F(B) &\leq F_{\max}(B_{n,\Delta}) = n_1 + 2^3 n_2 + \dots + \Delta^3 n_{\Delta} \\ &= (\Delta - 1)k + p - 1 + 2(\Delta - 1)^3 + \Delta^3(k - 1) \\ &= (\Delta^3 + \Delta - 1)k + p + \Delta^3 - 6\Delta^2 + 6\Delta - 3 \\ &= (\Delta^3 + \Delta - 1)k + p + (\Delta - 2)(\Delta^2 - 4\Delta - 2) - 7 \\ &= (\Delta^3 + \Delta - 1)k + p + (p + 3)(\Delta^2 - 4\Delta - 2) - 7 \\ &= (\Delta^2 + \Delta + 2)n - p(5\Delta + 3) + 3\Delta^2 - 12\Delta - 13 \\ &< (\Delta^2 + \Delta + 2)n - p(\Delta^2 + \Delta + 2) + p^3 + 9p^2 + 28p + 26. \end{aligned}$$

since

$$-p(5\Delta + 3) + 3\Delta^2 - 12\Delta - 13 < -p(\Delta^2 + \Delta + 2) + p^3 + 9p^2 + 28p + 26.$$

Subcase 2.3 $p + 3 \leq \Delta - 3$.

Then $n_2 + 2n_3 + \dots + n_{\Delta-1} = (\Delta - 2) + (p + 3)$. Therefore

$$(n_1, n_2, \dots, n_{p+4}, \dots, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k + p - 1, 0, \dots, 0, 1, \dots, 0, 1, k - 1)$$

which is the optimal solution and $p \leq \Delta - 4$ and $\Delta \geq 5$, then we have

$$\begin{aligned} F(B) &\leq F_{\max}(B_{n,\Delta}) = n_1 + 2^3 n_2 + \dots + \Delta^3 n_{\Delta} \\ &= (\Delta - 2)k + p - 1 + (p + 4)^3 + \Delta^3 - 3\Delta^2 + 3\Delta - 1 + \Delta^3(k - 1) \\ &= (\Delta^3 + \Delta - 2)k + p + (p + 4)^3 - 3\Delta^2 + 3\Delta - 2 \\ &= (\Delta^2 + \Delta + 2)n - p(\Delta^2 + \Delta + 2) + p^3 + 12p^2 + 49p - 3\Delta^2 + 3\Delta + 62 \\ &< (\Delta^2 + \Delta + 2)n - p(\Delta^2 + \Delta + 2) + p^3 + 9p^2 + 28p + 26, \end{aligned}$$

since for $\Delta \geq 3$, $p^3 + 12p^2 + 49p - 3\Delta^2 + 3\Delta + 62 < p^3 + 9p^2 + 28p + 26$.

Case 3. $2 \leq r < \Delta - p - 1$.

By (4), we have $n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)r + (p + r + 2)$. Since $r < \Delta - p - 1$, it follows from Corollary 1 that

$$(n_1, n_2, \dots, n_{p+r+3}, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k + p - 1, 0, \dots, 0, 1, 0, \dots, 0, r, k - r)$$

which is the optimal solution. On the other hand, we deduce from $p \leq \Delta - 3$ and $r < \Delta - p - 1$ and $\Delta \geq 6$. Thus

$$\begin{aligned}
F(B) &\leq n_1 + 2^3 n_2 + \dots + (\Delta - 1)^3 n_{\Delta-1} + \Delta^3 n_{\Delta} \\
&= (\Delta - 2)k + p - 1 + (p + r + 3)^3 + (\Delta - 1)^3 r + \Delta^3 (k - r) \\
&= (\Delta^3 + \Delta - 2)k + p - 1 + (p^3 + (r + 3)^3 + 3p^2(r + 3) + 3p(r + 3)^2) - 3\Delta^2 r + 3\Delta r - r \\
&= (\Delta^3 + \Delta - 2)k + p^3 + 9p^2 + 28p - 1 + (r + 3)^3 + 3pr(p + r + 2) - 3\Delta^2 r + 3\Delta r - r \\
&< (\Delta^3 + \Delta - 2)k + p^3 + 9p^2 + 28p + 26 + r^3 + 9r^2 + 27r + 3pr(\Delta + 1) - 3\Delta^2 r + 3\Delta r - r \\
&= (\Delta^3 + \Delta - 2)k + p^3 + 9p^2 + 28p + 26 + r(r(r + 9) + 27 + 3p(\Delta + 1) - 3\Delta^2 + 3\Delta - 1) \\
&< (\Delta^3 + \Delta - 2)k + p^3 + 9p^2 + 28p + 26 + r((\Delta - p - 1)(\Delta - p + 8) + 26 + 3p(\Delta + 1) \\
&\quad - 3\Delta^2 + 3\Delta) \\
&= (\Delta^3 + \Delta - 2)k + p^3 + 9p^2 + 28p + 26 + r(-2\Delta^2 + 10\Delta + p\Delta + p(p - 4) + 18) \\
&< (\Delta^3 + \Delta - 2)k + p^3 + 9p^2 + 28p + 26 + r(-2\Delta^2 + 10\Delta + \Delta(\Delta - 3) \\
&\quad + (\Delta - 3)(\Delta - 7) + 18) \\
&= (\Delta^2 + \Delta + 2)(n - p) + p^3 + 9p^2 + 28p + 26 + r(-3\Delta + 39) \\
&< (\Delta^2 + \Delta + 2)(n - p) + p^3 + 9p^2 + 28p + 26.
\end{aligned}$$

Case 4. $\Delta - p - 1 \leq r \leq k - 1$.

Let $p + r = t(\Delta - 2) + s$. By substituting in (4), we have

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)(r + t) + s.$$

If $s = 0$ then by Corollary 1,

$$(n_1, n_2, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k + p - (t + 1), 0, 1, 0, \dots, 0, r + t, k - r)$$

which is the optimal solution. Since $\Delta - p \leq r + 1$ and $p < \Delta - 3$, and clearly

$$\Delta^3 - 9\Delta^2 + 10\Delta - 6 < p^3 + 9p^2 + 26p + 1 < \Delta^3 - \Delta - 23.$$

Thus

$$\begin{aligned}
F(B) &\leq n_1 + 2^3 n_2 + \dots + (\Delta - 1)^3 n_{\Delta-1} + \Delta^3 n_{\Delta} \\
&= (\Delta - 2)k + p - (t + 1) + (3)^3 + (\Delta - 1)^3 (t + r) + \Delta^3 (k - r) \\
&= (\Delta^3 + \Delta - 2)k + p + 26 + \Delta^3 t - 3\Delta^2 t + 3\Delta t - 2t - 3\Delta^2 r + 3\Delta r - r
\end{aligned}$$

$$\begin{aligned}
&= (\Delta^3 + \Delta - 2)k + p + 26 - t(\Delta^3 + 3\Delta^2 - 3\Delta + 2) - r(3\Delta^2 - 3\Delta + 1) \\
&< (\Delta^3 + \Delta - 2)k + p + 26 - 1(\Delta^3 + 3\Delta^2 - 3\Delta + 2) + (p - \Delta + 1)(3\Delta^2 - 3\Delta + 1) \\
&= (\Delta^3 + \Delta - 2)k + p + 26 + p(3\Delta^2 - 3\Delta + 1) + 2\Delta^3 - 3\Delta^2 - \Delta + 25 \\
&= (\Delta^2 + \Delta + 2)n - p(-2\Delta^2 + 4\Delta - 2) - 2\Delta^3 + 3\Delta^2 - \Delta + 25 \\
&< (\Delta^2 + \Delta + 2)n - p(\Delta^2 + \Delta + 2) + p^3 + 9p^2 + 28p + 26.
\end{aligned}$$

Now let $0 < s$. Since $s < \Delta - 2$, it follows from Corollary 1 that

$$(n_1, n_2, \dots, n_s, n_{s+1}, n_{s+2}, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta-2)k+p-(t+1), 0, \dots, 0, 1, 0, \dots, 0, 0, r+t, k-r)$$

which is the optimal solution. Since $2 \leq p < \Delta - 3$ and $0 < s \leq \Delta - 3$ and clearly $-p(-2\Delta^2 + 4\Delta - 2) - \Delta^3 + 3\Delta^2 - \Delta - 2 < 2\Delta^3 - 15\Delta^2 + 10\Delta - 6 < p^3 + 9p^2 + 28p + 26$.

Thus

$$\begin{aligned}
F(B) &\leq n_1 + 2^3n_2 + \dots + (\Delta - 1)^3n_{\Delta-1} + \Delta^3n_{\Delta} \\
&= (\Delta - 2)k + p - (t + 1) + (s + 3)^3 + (\Delta - 1)^3(t + r) + \Delta^3(k - r) \\
&= (\Delta^3 + \Delta - 2)k + p - 1 + (s + 3)^3 - t(-\Delta^3 + 3\Delta^2 - 3\Delta + 2) - r(3\Delta^2 - 3\Delta + 1) \\
&< (\Delta^3 + \Delta - 2)k + p - 1 + \Delta^3 - 1(-\Delta^3 + 3\Delta^2 - 3\Delta + 2) + (p + 1 - \Delta)(3\Delta^2 - 3\Delta + 1) \\
&= (\Delta^2 + \Delta + 2)n - p(-\Delta^2 + \Delta + 2) + p + p(3\Delta^2 + 3\Delta + 1) - \Delta^3 + 3\Delta^2 - \Delta - 2 \\
&= (\Delta^2 + \Delta + 2)n - p(-2\Delta^2 + 4\Delta - 2) - \Delta^3 + 3\Delta^2 - \Delta - 2 \\
&< (\Delta^2 + \Delta + 2)n - p(\Delta^2 + \Delta + 2) + p^3 + 9p^2 + 28p + 26.
\end{aligned}$$

This completes the proof. □

Funding Information: J. Rodríguez was supported by MINEDUC-UA project, code ANT-1899 and Funded by the Initiation Program in Research - Universidad de Antofagasta, INI-19-06.

References

- [1] H. Abdo, D. Dimitrov, I. Gutman, On extremal trees with respect to the F-index, Kuwait J. Sci. 44 (3) (2017) 1-8.

- [2] S. Akhter, M. Imran, M. Farahani, Extremal unicyclic and bicyclic graphs with respect to the F-index, *AKCE Int. J. Graphs Comb.* 14 (2017) 80-91.
- [3] B. Basavanagoud, S. Timmanaikar, Computing first Zagreb and forgotten indices of certain dominating transformation graphs of Kragujevac trees, *Journal of Computer and Mathematical Sciences.* 8 (2017), 50-61.
- [4] Z. Che, Z. Chen, Lower and upper bounds of the forgotten topological index, *MATCH Commun. Math. Comput. Chem.* 76 (2016), 635-648.
- [5] S. Elumalai, T. Mansour, M. Rostami, On the bounds of the forgotten topological index, *Turk. J. Math.* 41 (2017) 1687-1702.
- [6] B. Furtula, I. Gutman, A forgotten topological index , *J. Math. Chem.* 53 (2015), 1184-1190.
- [7] W. Gao, M.R. Farahani, L. Shi, Forgotten topological index of some drug structures, *Acta Med. Medit.*, 32 (1) (2016) 579-585.
- [8] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. Total π -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* 17 (1972), 535-538.
- [9] M. Javaid, M. Ahmad, M. Hussain, W.C. Teh, Bounds of F-index for unicyclic graphs with fixed pendent vertices, *Journal of Prime Research in Mathematics* 14 (2018) 51-61.
- [10] A. Khaksari, M. Ghorbani, On the forgotten topological index, *Iranian J. Math. Chem.* 8 (2017), 1-12.
- [11] I.Z. Milovanović, M.M. Matejić, E.I. Milovanović, Remark on forgotten topological index of line graphs, *Bull. IMVI* 7 (2017) 473-478.
- [12] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.
- [13] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley-VCH, Weinheim, 2009.