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Extremal reformulated forgotten index of trees, unicyclic and bicyclic graphs

Ishita Sarkar[a], Manjunath Nanjappa[a], Ivan Gutman[b]

[a] *Department of Mathematics, CHRIST (Deemed to be University), Bengaluru 560029, India*
[b] *Faculty of Science, University of Kragujevac, 34000 Kragujevac, Serbia*

Abstract. The reformulated forgotten index (RF) is the edge version of the ordinary forgotten index. We describe graph transformations, by means of which RF increases or decreases. Using these transformations, the trees, unicyclic, and bicyclic graphs extremal w.r.t. RF are characterized.

1. Introduction

Throughout this paper, only connected, simple, undirected graphs are considered. Let H be such a graph. Then $V(H)$ and $E(H)$ denote its vertex and edge sets, respectively, and $e = vw$ is the edge joining the vertices v with w. The set consisting of the vertex $w \in V(H)$ and the vertices adjacent to w is denoted by $N_H(w)$.

The number of edges incident on a vertex w is the degree of w, denoted by $d_H(w)$. The degree of an edge e, denoted by $d_H(e)$, is the number of edges incident to e. Recall that $d_H(e) = d_H(v) + d_H(w) - 2$.

Topological indices are an important auxiliary means used to relate molecular structure with physico-chemical characteristics of chemical compounds, especially those relevant for their pharmacological, medicinal, toxicological, and similar properties. The Zagreb indices, defined as

$$M_1(H) = \sum_{w \in V(H)} d_H(w)^2 = \sum_{vw \in E(H)} \left[d_H(v) + d_H(w)\right]$$

and

$$M_2(H) = \sum_{vw \in E(H)} d_H(v)\, d_H(w)$$

are two of the oldest and most thoroughly examined molecular descriptors of this kind [3, 8–10]. Numerous variants these indices were put forward, for details see [9]. Among these are the so-called "reformulated Zagreb indices" [14]

$$EM_1(H) = \sum_{e \in E(H)} d_H(e)^2 = \sum_{e \sim f \in E(H)} \left[d_H(e) + d_H(f)\right]$$

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Email addresses: ishita.sarkar@res.christuniversity.in (Ishita Sarkar), manjunath.nanjappa@christuniversity.in (Manjunath Nanjappa), gutman@kg.ac.rs (Ivan Gutman)

and

$$EM_2(H) = \sum_{e \sim f \in E(H)} d_H(e)\, d_H(f)\,.$$

It is easy to see that the reformulated Zagreb index of the graph H coincides with the ordinary Zagreb index of the line graph of H.

Another extension of the Zagreb-index concept is the "forgotten" topological index [7]

$$F(H) = \sum_{w \in V(H)} d_H(w)^3 = \sum_{vw \in E(H)} \left[d_H(v)^2 + d_H(w)^2 \right]$$

which also has been much studied [1, 4, 5, 12]. In this paper we are concerned with the reformulated version of the forgotten index, namely with

$$RF(H) = \sum_{e \in E(H)} d_H(e)^3 = \sum_{e \sim f} \left[d_H(e)^2 + d_H(f)^2 \right].$$

Evidently, $RF(H)$ is just the ordinary forgotten index of the line graph of H.

The study on RF-index was initiated by Aram and Dehgardi in [2]. Other works on this graph invariant are found in [13, 15]. Here we characterize the trees, unicyclic, and bicyclic graphs extremal w.r.t. RF. In order to achieve this goal, we construct a number of auxiliary transformations.

2. Transformations increasing the reformulated forgotten index

This section discusses certain operations on graphs [6, 11, 16] that increase the reformulated forgotten index

Transformation 1: Assume that H_0 is a non trivial graph and $b \in V(H_0)$. Construct H_1 from H_0 by joining b with the central node of star where, $d_{H_1}(c) \geq 2$. Also, $z_1, z_2, z_3, \ldots z_t$ are the vertices adjacent to c, which are also pendent vertices in H_1. We now apply transformation 1 on H_1 to obtain H_2 where $H_2 = H_1 - \{cz_i\} + \{bz_i\}$, $i = 1, 2, \ldots, t$, see Fig. 1.

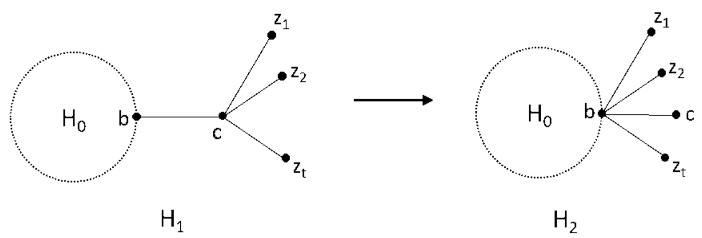


Figure 1: Transformation 1

Lemma 2.1. *Assume that H_2 is generated by transformation 1 on H_1. Then, $RF(H_1) < RF(H_2)$.*

Proof. We know that $d_{H_1}(b) < d_{H_2}(b)$ and $d_{H_1}(bc) = d_{H_2}(bc)$. Then,

$$\begin{aligned} RF(H_2) - RF(H_1) &> \sum_{i=1}^{t} \left[d_{H_2}(bz_i)^3 - d_{H_1}(cz_i)^3 \right] + d_{H_2}(bc)^3 - d_{H_1}(bc)^3 \\ &= \sum_{i=1}^{t} \left[d_{H_2}(bz_i)^3 - d_{H_1}(cz_i)^3 \right] > 0\,. \end{aligned}$$

$\Longrightarrow RF(H_1) < RF(H_2)\,.$

□

Transformation 2: Let for $b, c \in V(H_1)$, there exists a path of length $t \geq 1$, joining b and c, as shown in Fig. 2. Then by applying transformation 2 on H_1, we obtain H_2 where $H_2 = H_1 - \{bb_1, b_1b_2, \ldots, b_{t-1}b_t(b_{t-1}c)\} + \{zb_1, zb_2, \ldots, zb_{t-1}\}$; $z = b \circ c$.

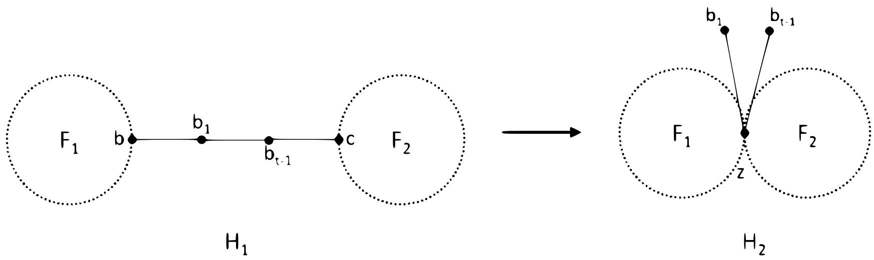


Figure 2: Transformation 2

Lemma 2.2. *Assume that H_2 is generated by the application of transformation 2 on H_1, Then, $RF(H_1) < RF(H_2)$.*

Proof. Let $d_{F_1}(b) = m \geq 1$ and $d_{F_2}(c) = n \geq 1$. We have $d_{H_2}(z) = m + n + t - 1$ where $t \geq 2$. If $t = 2$, then $RF(H_2) - RF(H_1) > d_{H_2}(b_1z)^3 - (m+n)^3 = (m+n)^3 - (m+n)^3 = 0$. Now, when $t \geq 3$, by the definition of RF index,

$$\begin{aligned}
RF(H_2) - RF(H_1) &> \sum_{i=1}^{t-1} d_{H_2}(zb_i)^3 - \Big[(m+1)^3 + (n+1)^3 + 8(t-3)\Big] \\
&= (t-1)(m+n+t-2)^3 - (m+1)^3 - (n+1)^3 - 8(t-3) \\
&> \Big[(m+n+t-2)^3 - (m+1)^3\Big] + \Big[(m+n+t-2)^3 - (n+1)^3\Big] \\
&> 0\,. \\
\implies RF(H_1) &< RF(H_2)\,.
\end{aligned}$$

□

Transformation 3: For $b, c \in V(H_0)$, we attache pendent vertices $\{b_1, b_2, \ldots, b_r\}$ and $\{c_1, c_2, \ldots, c_t\}$ to b and c, respectively, obtaining H_1 from H_0. Thus, applying two possibilities of transformation 3 on H_1, we obtain H_2 and H_3 where $H_2 = H_1 + \{cb_1, cb_2, \ldots, cb_r\} - \{bb_1, bb_2, \ldots bb_r\}$ and $H_3 = H_1 + \{bc_1, bc_2, \ldots, bc_t\} - \{cc_1, cc_2, \ldots cc_t\}$, see Fig. 3.

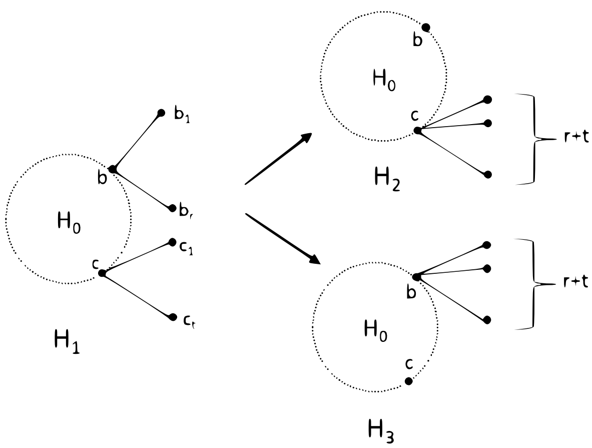


Figure 3: Transformation 3

Lemma 2.3. *Assume that H_2 and H_3 are generated by application of transformation 3 on H_1. Then either $RF(H_1) < RF(H_3)$ or $RF(H_1) < RF(H_2)$.*

Proof. Let us assume $d_{H_0}(b) = p$, $d_{H_0}(c) = q$ for $p, q > 0$. For $r, t \geq 1$, by the definition of $RF-$ index,

$$\begin{aligned}
RF(H_2) - RF(H_1) &> \sum_{i=1}^{r} d_{H_2}(cb_i)^3 - \sum_{i=1}^{r} d_{H_1}(bb_i)^3 + \sum_{i=1}^{t} d_{H_2}(cc_i)^3 - \sum_{i=1}^{t} d_{H_1}(cc_i)^3 \\
&= (q + t - p) \sum_{i=1}^{r} \left(d_{H_2}(cb_i)^2 + d_{H_2}(cb_i) d_{H_1}(bb_i) + d_{H_1}(bb_i)^2 \right) \\
&+ r \sum_{i=1}^{t} \left(d_{H_2}(cc_i)^2 + d_{H_2}(cc_i) d_{H_1}(cc_i) + d_{H_1}(cc_i)^2 \right) \\
&> (r + t + q - p) \\
RF(H_3) - RF(H_1) &> \sum_{i=1}^{r} d_{H_3}(bb_i)^3 - \sum_{i=1}^{r} d_{H_1}(bb_i)^3 + \sum_{i=1}^{t} d_{H_3}(bc_i)^3 - \sum_{i=1}^{t} d_{H_1}(cc_i)^3 \\
&= t \sum_{i=1}^{r} \left(d_{H_3}(bb_i)^2 + d_{H_3}(bb_i) d_{H_1}(bb_i) + d_{H_1}(bb_i)^2 \right) \\
&+ (p + r - q) \sum_{i=1}^{t} \left(d_{H_3}(bc_i)^2 + d_{H_3}(bc_i) d_{H_1}(cc_i) + d_{H_1}(cc_i)^2 \right) \\
&> (r + t + p - q) \, .
\end{aligned}$$

If $p > q$, then $RF(H_3) > RF(H_1)$ holds true, but $RF(H_2) > RF(H_1)$ may or may not hold. Similarly if $q > p$, then $RF(H_2) > RF(H_1)$ holds true, but $RF(H_3) > RF(H_1)$ may or may not hold. If $p = q$, then both conditions $RF(H_2) > RF(H_1)$ and $RF(H_3) > RF(H_1)$ certainly holds true. □

3. Transformations decreasing the reformulated forgotten index

This section describes three operations on graphs [6, 11, 16] that decrease the RF-index.

Transformation 4: Assume that H_0 is a non-trivial graph and $b \in V(H_0)$. We obtain H_1 from H_0 by attaching two paths to b, $P_1 = bb_1b_2 \ldots b_r$ and $P_2 = bc_1c_2 \ldots c_t$. By transformation 4, H_1 is changed to H_2 where $H_2 = H_1 + \{c_tb_1\} - \{bb_1\}$, see Fig. 4.

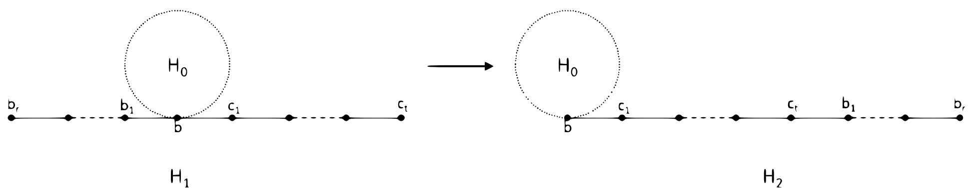


Figure 4: Transformation 4

Lemma 3.1. *Assume that H_2 is generated from H_1 by transformation 4. Then $RF(H_1) > RF(H_2)$.*

Proof. When $r, t \geq 3$, by the definition of $RF-$ index,

$$\begin{aligned}
RF(H_1) - RF(H_2) &> d_{H_1}(bb_1)^3 + d_{H_1}(bc_1)^3 + d_{H_1}(c_{t-1}c_t)^3 - \Big[d_{H_2}(c_tb_1)^3 + d_{H_2}(bc_1)^3 \\
&+ d_{H_2}(c_{t-1}c_t)^3 \Big] \\
&= 2(d_{H_0}(b) + 2)^3 + 1 - (d_{H_0}(b) + 1)^3 - 16 \\
&= d_{H_0}(b)^3 + 9d_{H_0}(b)^2 + 21d_{H_0}(b) > 0 \, .
\end{aligned}$$

Analogous results are obtained for other values of r and t i.e., $r = 1, t = 1$; $r = 1, t = 2$; $r = 2, t = 2$; $r = 1, t \geq 3$; $r = 2, t \geq 3$. We skip the details. □

Transformation 5: Assume that H_0 is a non-trivial graph and $b, c \in V(H_0)$. We obtain H_1 from H_0 by attaching a path to b and another to c; $P_1 = bb_1b_2 \ldots b_r$ (length r) and $P_2 = cc_1c_2 \ldots c_t$ (length t). By transformation 5, H_1 is changed to H_2 where $H_2 = H_1 + \{bb_1\} - \{c_tb_1\}$, see Fig. 5.

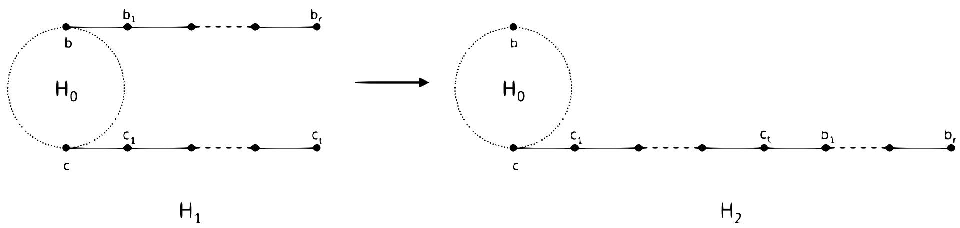


Figure 5: Transformation 5

Lemma 3.2. *Assume that H_2 is generated from H_1 by transformation 5. Then $RF(H_1) > RF(H_2)$.*

Proof. We know $d_{H_1}(bb_1) \geq 3$, for $r, t \geq 3$, by definition of $RF-$ index,

$$\begin{aligned} RF(H_1) - RF(H_2) &> d_{H_1}(bb_1)^3 + 1 + 8(r-2) + (d_{H_0}(c)+1)^3 + 1 + 8(t-2) \\ &\quad - \left(d_{H_0}(c)+1)^3 + 8(r+t-2) + 1\right) \\ &= d_{H_1}(bb_1)^3 - 15 > 0\,. \\ \Longrightarrow RF(H_1) &> RF(H_2) \end{aligned}$$

Analogous results are obtained for other values of r and t i.e., $r = 2, t = 3$; $r = 2, t = 2$; $r = 1, t = 3$; $r = 1, t = 2$. We skip the details. □

Transformation 6: Assume that the graph H_0 contains a path between vertices b and c of length at least 2, and x_1 is a vertex lying on this path, e.g. $< b, x_1, c >$. We obtain H_1 from H_0 by attaching a path to vertex x_1, for $k \geq 1$, $< x_1, x_2 \ldots x_k >$ (see Fig. 6). By using transformation 6, H_1 is changed to H_2 where $H_2 = H_1 + \{x_kv\} - \{x_1v\}$, see Fig. 6.

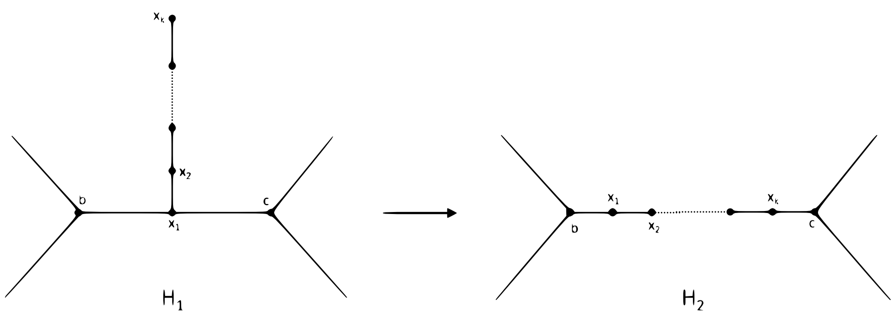


Figure 6: Transformation 6

Lemma 3.3. *Assume that H_2 is generated from H_1 by transformation 6. Then $RF(H_1) > RF(H_2)$.*

Proof. We know from the figure 6, $d_{H_1}(x_1c) - 1 = d_{H_2}(x_kc)$, $d_{H_1}(bx_1) - 1 = d_{H_2}(bx_1)$ and by the definition of RF

index;

$$
\begin{aligned}
RF(H_1) - RF(H_2) &> d_{H_1}(x_{k-1}x_k)^3 + d_{H_1}(x_1x_2)^3 + d_{H_1}(bx_1)^3 + d_{H_1}(cx_1)^3 - \Big[d_{H_2}(x_{k-1}x_k)^3 \\
&\quad + d_{H_2}(x_1x_2)^3 + d_{H_2}(bx_1)^3 + d_{H_2}(cx_k)^3\Big] \\
&= (d_{H_1}(b)+1)^3 + (d_{H_1}(c)+1)^3 - d_{H_1}(b)^3 - d_{H_1}(c)^3 + 12 > 0\,.
\end{aligned}
$$

Lemma 3.3 follows. □

4. Graphs with extremal reformulated forgotten index

In this section, by using the above described transformations, we determine the trees, unicyclic, and bicyclic graphs, extremal with respect to the reformulated forgotten index.

4.1. Extremal trees

Theorem 4.1. *Let T is a tree of order $n \geq 4$ distinct from P_n and S_n. Then*

$$2(4n-11) = RF(P_n) < RF(T) < RF(S_n) = (n-1)(n-2)^3\,.$$

Proof. The star graph S_n can be obtained from a tree T by utilizing the transformations 1 and 3. Therefore, $RF(T) < RF(S_n)$ holds true by Lemmas 2.1 and 2.3. The path graph P_n can be obtained from a tree T by repeated applications of transformation 4. Thus, $RF(P_n) < RF(T)$. By direct computation, we get $RF(S_n) = (n-1)(n-2)^3$ and $RF(P_n) = 2(4n-11)$. Thus, the trees with a fixed order n, with minimal and maximal RF index are P_n and S_n, respectively. □

4.2. Extremal unicyclic graphs

Let U_n^j be the unicyclic graph obtained by attaching $n-j$ pendent vertices to a vertex of the cycle C_j.

Theorem 4.2. *Let H be a unicyclic graph of order n and girth j. Then $RF(U_n^j) \geq RF(H)$ with equality iff $H \cong U_n^j$.*

Proof. We get U_n^j from H by transformations 1 and 3. Theorem 4.2 follows now from Lemmas (2.1) and (2.3). □

By direct calculation,

$$RF(U_n^j) = (n-j)(n-j+1)^3 + 2(n-j+2)^3 + 8(j-4)\,,$$

and therefore

$$
\begin{aligned}
RF(U_n^j) - RF(U_n^{j-1}) &= -(n-j-1)(n-j+2)^3 + (n-j)(n-j+1)^3 - 2(n-j+3)^3 + 8 \\
&\leq 0\,.
\end{aligned}
$$

This implies:

Corollary 4.3. *If $4 \leq j \leq n$, then $RF(U_n^{j-1}) \geq RF(U_n^j)$.*

Corollary 4.4. *Among all unicyclic graphs of order n, U_n^3 has uniquely the largest value of the RF index.*

Let C_n^j be the "tadpole" graph, obtained by attaching a path of order $n-j$ to a vertex of the cycle C_j.

Theorem 4.5. *Let H be a unicyclic graph distinct from C_n and C_n^j, $n-j = 1, 2, \ldots, n-3$. Then for $j \leq n-2$,*

$$RF(C_n) < RF(C_n^{n-1}) < RF(C_n^j) < RF(H)\,.$$

Proof. By direct calculation it can be shown that for $n-j \geq 2$, all graph $RF(C_n^j)$ have equal RF-values, and that C_n^{n-1}, i.e, when $n-j=1$, the RF-value is smaller than for other C_n^j-graphs. Theorem 4.5 follows now directly from Lemmas 3.1, 3.2 and 3.3. □

4.3. Extremal bicyclic graphs

Denote by $\mathbb{B}(p, p+1)$ the set of (connected) bicyclic graphs having p vertices and $p+1$ edges. There are three types of such bicyclic graphs, $\mathbb{B}^1_p(m,n)$, $\mathbb{B}^2_p(m,n,h)$, and $\mathbb{B}^3_p(m,n,h)$.

(i) For $\mathbb{B}^1_p(m,n) \subset \mathbb{B}(p,p+1)$, $m+n-1 \le p$. A graph belongs to $\mathbb{B}^1_p(m,n)$ if the cycles of length m and n are joined by a common vertex. Fig 7, depicts the graphs $D^1_p(m,n)$ with exactly $p = m+n-1$ vertices.

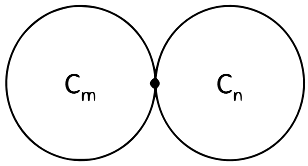


Figure 7: $D^1_p(m,n)$

(ii) For $\mathbb{B}^2_p(m,n,h) \subset \mathbb{B}(p,p+1)$, $m+n+h-1 \le p$. A graph belongs to $\mathbb{B}^2_p(m,n,h)$ if two cycles of length m and n are connected by P_{h+1} , $h \ge 1$. Fig. 8 depicts the graphs $D^2_p(m,n,h)$ with exactly $p = m+n+h-1$ vertices.

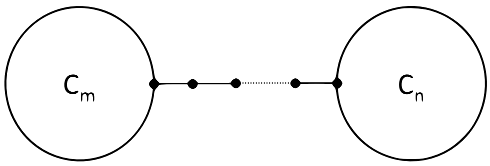


Figure 8: $D^2_p(m,n,h)$

(iii) For $\mathbb{B}^3_p(m,n,h) \subset \mathbb{B}(p,p+1)$, $m+n-h-1 \le p$. A graph belonging to $\mathbb{B}^3_p(m,n,h)$ if the cycles of length m and n have a common path, P_{h+1} , $h \ge 1$. Fig. 9 depicts the $D^3_p(m,n,h)$ with exactly $p = m+n-h-1$ vertices.

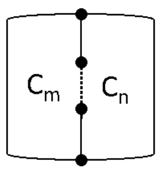
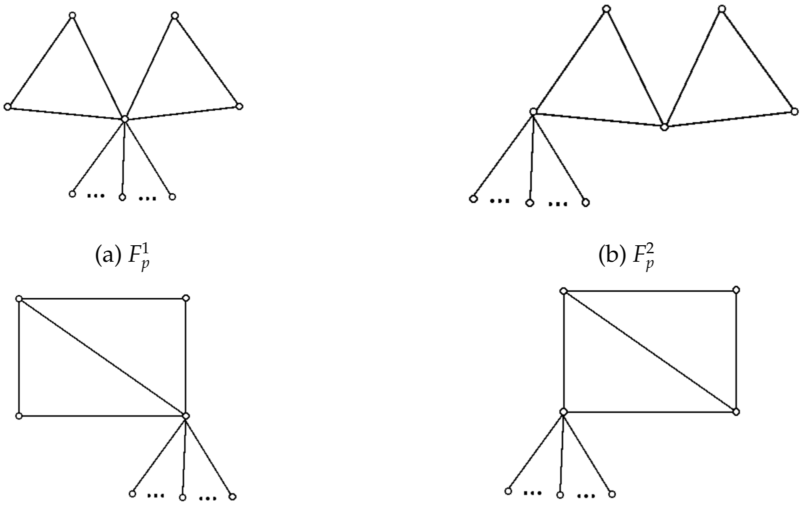


Figure 9: $D^3_p(m,n,h)$

Theorem 4.6. *The unique extremal graph among bicyclic graphs with maximal reformulated forgotten index is F^3_p, depicted in Fig. 10.*

Proof. Let H belong to one of the three above mentioned classes of bicyclic graphs. Suppose that $H \in \mathbb{B}^1_p(m,n)$ or $H \in \mathbb{B}^2_p(m,n,h)$. Then by repeated applications of transformations 1, 2, and 3 on H, we arrive at F^1_p or F^2_p, see Fig. 10. By Lemmas 2.1, 2.2 and 2.3, $RF(F^1_p) \ge RF(H)$ or $RF(F^2_p) \ge RF(H)$.



(a) F_p^1 (b) F_p^2

(c) F_p^3 (d) F_p^4

Figure 10: Bicyclic Graphs used for the maximal extremal graph

Suppose now that $H \in \mathbb{B}_p^3(m,n,h)$. By repeated applications of transformations 1, 2, and 3, one arrives at F_p^3 or F_p^4, see Fig. 10. Then by Lemmas 2.1, 2.2 and 2.3, we get $RF(F_p^3) \geq RF(H)$ or $RF(F_p^4) \geq RF(H)$.
Direct computation yields

$$RF(F_p^1) = p^4 - 7p^3 + 30p^2 - 56p + 52 \ ; \ RF(F_p^3) = p^4 - 7p^3 + 30p^2 - 50p + 84$$
$$RF(F_p^2) = p^4 - 15p^3 + 96p^2 - 274p + 492 \ ; \ RF(F_p^4) = p^4 - 11p^3 + 57p^2 - 129p + 224\,.$$

Comparing these results we arrive at Theorem 4.6. □

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