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A Unified Approach to the Extremal Zagreb Indices for Trees, Unicyclic Graphs and Bicyclic Graphs[1]

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Abstract

For a (molecular) graph, the first Zagreb index M_1 is equal to the sum of the squares of the degrees of the vertices, and the second Zagreb index M_2 is equal to the sum of the products of the degrees of pairs of adjacent vertices. This paper presents a unified and simple approach to the largest and smallest Zagreb indices for trees, unicyclic graphs and bicyclic graphs by introducing some transformations, and characterize these graphs with the largest and smallest Zagreb indices, respectively.

1 Introduction

Let $G = (V, E)$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. The first Zagreb index M_1 and the second Zagreb index

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M_2 of G are defined as

$$M_1(G) = \sum_{x \in V(G)} (d_G(x))^2$$

$$M_2(G) = \sum_{xy \in E(G)} d_G(x) d_G(y)$$

where $d_G(x)$ is the degree of vertex x in G.

The Zagreb indices M_1 and M_2 were introduced in [1] and elaborated in [2]. The main properties of M_1 and M_2 were summarized in [3,4]. These indices reflect the extent of branching of the molecular carbon-atom skeleton, and can thus be viewed as molecular structure-descriptors [5,6].

Recently, finding the extremal values or bounds for the topological indices of graphs, as well as related problems of characterizing the extremal graphs, attracted the attention of many researchers and many results are obtained (see [3-16]). [4] showed that the trees with the smallest and largest M_1 are the path and the star, respectively. [7] also showed that the trees with the smallest and largest M_2 are the path and the star, respectively. [15] characterized the graphs with the smallest and largest M_2 among all unicyclic graphs. [9] gave the the unicyclic graphs with the first three smallest and largest M_1. [16] gave the bicyclic graph with the largest M_1.

In this paper, we present a unified and simple approach to the largest and smallest Zagreb indices for trees, unicyclic graphs and bicyclic graphs by introducing some transformations, and characterize these graphs with the extremal Zagreb indices. The results which characterize the bicyclic graphs with extremal M_2 are new.

2 Two transformations which increase the Zagreb indices

For any $v \in V(G)$, $N_G(v) = \{u | uv \in E(G)\}$ denotes the neighbors of v, and $d_G(v) = |N_G(v)|$ is the degree of v in G.

Let $E' \subseteq E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E'. $W \subseteq V(G)$, $G - W$ denotes the subgraph of G obtained by deleting the vertices of W and the edges incident with them.

We give two transformations which will increase the Zagreb indices as follows:

Transformation A: Let uv be an edge G, $d_G(v) \geq 2$, $N_G(u) = \{v, w_1, w_2, \cdots, w_t\}$, and $w_1, w_2, \cdots, w_t$ are leaves. $G' = G - \{vw_1, vw_2, \cdots, vw_t\} + \{uw_1, uw_2, \cdots, uw_t\}$, as shown in Figure 1.

Lemma 2.1. Let G' be obtained from G by transformation A, then

$$M_1(G') > M_1(G) \text{ and } M_2(G') > M_2(G).$$

Proof. Let $G_0 = G - \{u, w_1, w_2, \cdots, w_t\}$. By the definition of the Zagreb indices, we have

$$\begin{aligned} M_1(G') - M_1(G) &= d^2_{G'}(v) - d^2_G(v) + d^2_{G'}(u) - d^2_G(u) \\ &= (d_G(v) + t)^2 - d^2_G(v) + 1 - (t+1)^2 \\ &= 2t(d_G(v) - 1) > 0 \end{aligned}$$

$$\begin{aligned} M_2(G') - M_2(G) &= \sum_{x \in N_{G_0}(v)} d_{G'}(v) d_{G'}(x) + (t+1) d_{G'}(v) \\ &\quad - \sum_{x \in N_{G_0}(v)} d_G(v) d_G(x) - (t+1) d_G(v) - t(t+1) \\ &= \sum_{x \in N_{G_0}(v)} (d_G(v) + t) d_G(x) + (t+1)(d_G(v) + t) \\ &\quad - \sum_{x \in N_{G_0}(v)} d_G(v) d_G(x) - (t+1) d_G(v) - t(t+1) \\ &= \sum_{x \in N_{G_0}(v)} t d_G(x) > 0 \end{aligned}$$

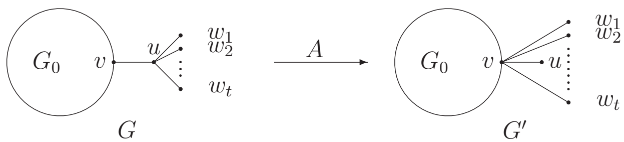


Figure 1. Transformation A.

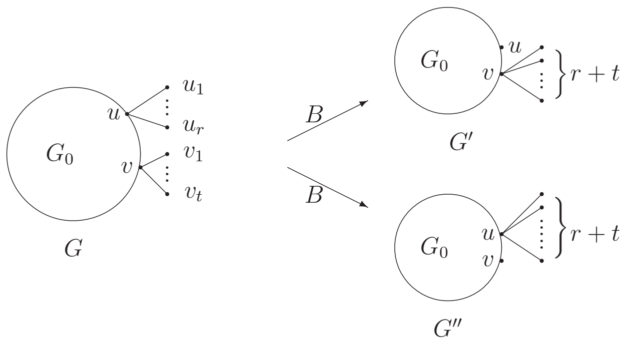


Figure 2. Transformation B.

Remark 1. Repeating Transformation A, any tree can changed into a star, any unicyclic or bicyclic graph can be changed into an unicyclic or bicyclic graph such that all the edges not on the cycles are pendant edges.

Transformation B: Let u and v be two vertices in G. $u_1, u_2, \cdots, u_r$ are the leaves adjacent to u, $v_1, v_2, \cdots, v_t$ are the leaves adjacent to v. $G' = G - \{uu_1, uu_2, \cdots, uu_r\} + \{vu_1, vu_2, \cdots, vu_r\}$, $G'' = G - \{vv_1, vv_2, \cdots, vv_t\} + \{uv_1, uv_2, \cdots, uv_t\}$, as showed in Figure 2.

Lemma 2.2. Let G' and G'' be obtained from G by transformation B, then either $M_i(G') > M_i(G)$ or $M_i(G'') > M_i(G)$, $i = 1, 2$.

Proof. Let $G_0 = G - \{u_1, u_2, \cdots, u_r, v_1, v_2, \cdots, v_t\}$.

$$\begin{aligned} M_1(G') - M_1(G) &= d^2_{G'}(v) - d^2_G(v) + d^2_{G'}(u) - d^2_G(u) \\ &= (d_G(v) + r)^2 - d^2_G(v) + (d_G(u) - r)^2 - d^2_G(u) \\ &= 2r(r + d_G(v) - d_G(u)) \end{aligned}$$

$$\begin{aligned} M_1(G'') - M_1(G) &= d^2_{G''}(v) - d^2_G(v) + d^2_{G''}(u) - d^2_G(u) \\ &= (d_G(v) - t)^2 - d^2_G(v) + (d_G(u) + t)^2 - d^2_G(u) \\ &= 2t(t + d_G(u) - d_G(v)) \end{aligned}$$

So, $M_1(G') > M_1(G)$ if $d_G(v) \geq d_G(u)$; otherwise $M_1(G'') > M_1(G)$.

Let $d_{G_0}(u) = p$ and $d_{G_0}(v) = q$.

(i) If u, v are not adjacent in G, then, by the definition of M_2, we have

$$\begin{aligned} M_2(G) = &\sum_{xy \in E(G_0 - \{u,v\})} d_{G_0}(x) d_{G_0}(y) + (p+r) \sum_{x \in N_{G_0}(u)} d_{G_0}(x) \\ &+ (q+t) \sum_{x \in N_{G_0}(v)} d_{G_0}(x) + r(p+r) + t(q+t) \end{aligned}$$

$$\begin{aligned} M_2(G') = &\sum_{xy \in E(G_0 - \{u,v\})} d_{G_0}(x) d_{G_0}(y) + p \sum_{x \in N_{G_0}(u)} d_{G_0}(x) \\ &+ (q+t+r) \sum_{x \in N_{G_0}(v)} d_{G_0}(x) + (r+t)(q+t+r) \end{aligned}$$

$$\begin{aligned} M_2(G'') = &\sum_{xy \in E(G_0 - \{u,v\})} d_{G_0}(x) d_{G_0}(y) + (p+r+t) \sum_{x \in N_{G_0}(u)} d_{G_0}(x) \\ &+ q \sum_{x \in N_{G_0}(v)} d_{G_0}(x) + (r+t)(p+r+t) \end{aligned}$$

$$\begin{aligned} \Delta_1 &= M_2(G') - M_2(G) \\ &= r\Big(\sum_{x \in N_{G_0}(v)} d_{G_0}(x) - \sum_{x \in N_{G_0}(u)} d_{G_0}(x)\Big) + r(2t + q - p) \\ \Delta_2 &= M_2(G'') - M_2(G) \\ &= t\Big(\sum_{x \in N_{G_0}(u)} d_{G_0}(x) - \sum_{x \in N_{G_0}(v)} d_{G_0}(x)\Big) + t(2r + p - q) \end{aligned}$$

If $\Delta_1 = M_2(G') - M_2(G) \leq 0$, then

$$\sum_{x \in N_{G_0}(u)} d_{G_0}(x) - \sum_{x \in N_{G_0}(v)} d_{G_0}(x) \geq 2t + q - p$$

So, $\Delta_2 = M_2(G'') - M_2(G) \geq t(2t+q-p) + t(2r+p-q) = 2t(t+r) > 0$.

(ii) If u, v are adjacent in G, then $u \in N_{G_0}(v)$ and $v \in N_{G_0}(u)$.

$$\begin{aligned} M_2(G) &= \sum_{xy \in E(G_0 - \{u,v\})} d_{G_0}(x) d_{G_0}(y) + (p+r) \sum_{x \in N_{G_0}(u)} d_{G_0}(x) \\ &\quad + (q+t) \sum_{x \in N_{G_0}(v)} d_{G_0}(x) + r(p+r) + t(q+t) - (p+r)(q+t) \end{aligned}$$

$$\begin{aligned} M_2(G') &= \sum_{xy \in E(G_0 - \{u,v\})} d_{G_0}(x) d_{G_0}(y) + p \sum_{x \in N_{G_0}(u)} d_{G_0}(x) \\ &\quad + (q+t+r) \sum_{x \in N_{G_0}(v)} d_{G_0}(x) + (r+t)(q+t+r) - p(q+t+r) \end{aligned}$$

$$\begin{aligned} M_2(G'') &= \sum_{xy \in E(G_0 - \{u,v\})} d_{G_0}(x) d_{G_0}(y) + (p+r+t) \sum_{x \in N_{G_0}(u)} d_{G_0}(x) \\ &\quad + q \sum_{x \in N_{G_0}(v)} d_{G_0}(x) + (r+t)(p+r+t) - q(p+r+t) \end{aligned}$$

$$\begin{aligned} \Delta_1 &= M_2(G') - M_2(G) \\ &= r\Big(\sum_{x \in N_{G_0}(v)} d_{G_0}(x) - \sum_{x \in N_{G_0}(u)} d_{G_0}(x)\Big) + r(3t+2q-2p) \\ \Delta_2 &= M_2(G'') - M_2(G) \\ &= t\Big(\sum_{x \in N_{G_0}(u)} d_{G_0}(x) - \sum_{x \in N_{G_0}(v)} d_{G_0}(x)\Big) + t(3r+2p-2q) \end{aligned}$$

If $\Delta_1 = M_2(G') - M_2(G) \leq 0$, then

$$\sum_{x \in N_{G_0}(u)} d_{G_0}(x) - \sum_{x \in N_{G_0}(v)} d_{G_0}(x) \geq 3t + 2q - 2p$$

So, $\Delta_2 = M_2(G'') - M_2(G) \geq t(3t+2q-2p) + t(3r+2p-2q) = 3t(t+r) > 0$.
The proof is completed.

Remark 2. Repeating Transformation B, any unicyclic or bicyclic graph can be changed into an unicyclic or bicyclic graph such that all the pendant edges are attached to the same vertex.

3 The graphs with the largest Zagreb indices

In this section, we give the tree, the unicyclic graph and the bicyclic graphs with the largest Zagreb indices.

From Lemma 2.1, we have

Theorem 3.1([4,7]). Let T be any tree of order n. If T is different from S_n, then $M_1(T) < M_1(S_n)$ and $M_2(T) < M_2(S_n)$.

Let U_n^k be the unicyclic graph obtained from the cycle C_k of length k by attached $n-k$ pendant edges to the same vertex on C_k. From Lemmas 2.1

and 2.2, we have

Theorem 3.2. Let G be an unicyclic graph of order n and girth k. If G is different from U_n^k, then $M_1(G) < M_1(U_n^k)$ and $M_2(G) < M_2(U_n^k)$.

Since $M_1(U_n^k) = 4(k-1)+(n-k+2)^2+4(k-1) = k^2-(2n+1)k+n^2+5n$ and $M_2(U_n^k) = k^2 - (2n+2)k + n^2 + 6n$, $M_1(U_n^k) \leq M_1(U_n^3)$ and $M_2(U_n^k) \leq M_2(U_n^3)$ for $3 \leq k \leq n$ with the equality if and only if $k = 3$. We have

Theorem 3.3([9,15]). U_n^3 is the unique graph with the largest Zagreb indices M_1 and M_2 among all unicyclic graphs with n vertices.

Now, we consider the $(n, n+1)-$graph (i.e., bicyclic graph with n vertices) and give the $(n, n+1)-$graph with the largest Zagreb indices.

Let $\mathcal{G}(n, n+1)$ be the set of simple connected graphs with n vertices and $n+1$ edges. For any graph $G \in \mathcal{G}(n, n+1)$, there are two cycles C_p and C_q in G. As in [16], we divide all the $(n, n+1)-$graphs with two cycles of lengths p and q into three classes.

(1) $\mathcal{A}(p, q)$ is the set of $G \in \mathcal{G}(n, n+1)$ in which the cycles C_p and C_q have only one common vertex;

(2) $\mathcal{B}(p, q)$ is the set of $G \in \mathcal{G}(n, n+1)$ in which the cycles C_p and C_q have no common vertex;

(3) $\mathcal{C}(p, q, l)$ is the set of $G \in \mathcal{G}(n, n+1)$ in which the cycles C_p and C_q have a common path of length l.

Note that the induced subgraph of vertices on the cycles of $G \in \mathcal{A}(p, q)$ (or $\mathcal{B}(p, q)$, $\mathcal{C}(p, q, l)$) is showed in Figure 3(a) (or (b),(c)) and $\mathcal{C}(p, q, l) = \mathcal{C}(p, p+q-2l, p-l) = \mathcal{C}(p+q-2l, q, q-l)$.

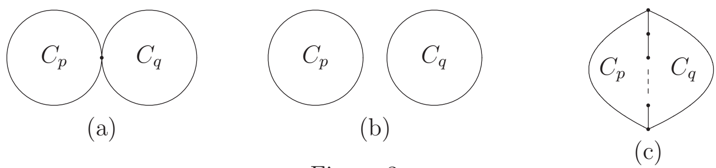
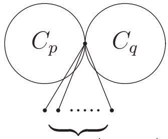


Figure 3.

First, we find the bicyclic graph with the largest Zagreb in $\mathcal{A}(p, q)$.

Let $S_n(p, q)$ be a graph in $\mathcal{A}(p, q)$ such that $n+1-(p+q)$ pendent edges are attached to the common vertex of C_p and C_q. See Figure 4.



$n+1-(p+q)$

Figure 4. The graph $S_n(p,q)$.

Theorem 3.4. (i) ([16]) $S_n(p,q)$ is the graph with the largest M_1 in $\mathcal{A}(p,q)$;

(ii) $S_n(p,q)$ is the graph with the largest M_2 in $\mathcal{A}(p,q)$.

Proof. First, repeating the transformations A and B on graph G, we can get a graph G' such that all the edges not on the cycles are the pendant edges attached to the same vertex v. By Lemmas 2.1 and 2.2, we have $M_1(G) \le M_1(G')$ and $M_2(G) \le M_2(G')$ with the equality if and only if all the edges not on the cycles are also the pendant edges attached to the same vertex in G. If $G' \ncong S_n(p,q)$, then $v \ne u$, where u is the common vertex of C_p and C_q.

Without loss of the generality, we assume that v is on the cycle C_p.

$$\begin{aligned}
& M_1(S_n(p,q)) - M_1(G') \\
= \;& (n+5-p-q)^2 + 4 - (n+3-p-q)^2 - 16 \\
= \;& 4(n+1-p-q) \ge 0
\end{aligned}$$

with the equality if and only if $n = p+q-1$, and $G' \cong S_n(p,q)$.

(i) If u and v are not adjacent (i.e., $k > 1$), then

$$\begin{aligned}
& M_2(S_n(p,q)) - M_2(G') \\
= \;& (n+5-p-q)(n+9-p-q) + 4(p-2) + 4(q-2) \\
& -(n+3-p-q)(n+5-p-q) - 4(p-4) - 4(q-2) - 32 \\
= \;& 6(n+1-p-q) \ge 0
\end{aligned}$$

with the equality if and only if $n = p+q-1$, and $G' \cong S_n(p,q)$.

(ii) If u and v are adjacent, then

$$\begin{aligned}
& M_2(S_n(p,q)) - M_2(G') \\
= \;& (n+5-p-q)(n+9-p-q) + 4(p-2) + 4(q-2) \\
& -(n+3-p-q)(n+7-p-q) - 4(p-3) - 4(q-2) - 24 \\
= \;& 4(n+1-p-q) \ge 0
\end{aligned}$$

with the equality if and only if $n = p+q-1$, and $G' \cong S_n(p,q)$.

Given $p \geq 3$ and $q \geq 3$, from the theorem above, we know $S_n(p, q)$ is the unique graph with the largest Zagreb indices in $\mathcal{A}(p, q)$.

Lemma 3.5. (i) If $p > 3$, then
$M_1(S_n(p, q)) < M_1(S_n(p-1, q))$ and $M_2(S_n(p, q)) < M_2(S_n(p-1, q))$;
(ii) If $q > 3$, then
$M_1(S_n(p, q)) < M_1(S_n(p, q-1))$ and $M_2(S_n(p, q)) < M_2(S_n(p, q-1))$.
Proof. From the symmetry of p and q, we only need to prove (i).

$$\begin{aligned} & M_1(S_n(p-1, q)) - M_1(S_n(p, q)) \\ = \; & (n+6-p-q)^2 + 1 - (n+5-p-q)^2 - 4 \\ = \; & 2(n+4-p-q) > 0 \end{aligned}$$

$$\begin{aligned} & M_2(S_n(p-1, q)) - M_2(S_n(p, q)) \\ = \; & (n+6-p-q)(n+10-p-q) - (n+5-p-q)(n+9-p-q) - 4 \\ = \; & 2(n+1-p-q) + 9 > 0 \end{aligned}$$

From Theorem 3.4 and Lemma 3.5, we know

Theorem 3.6. For all $p \geq 3$ and $q \geq 3$, $S_n(3, 3)$ is the unique graph with the largest Zagreb indices in $\mathcal{A}(p, q)$.

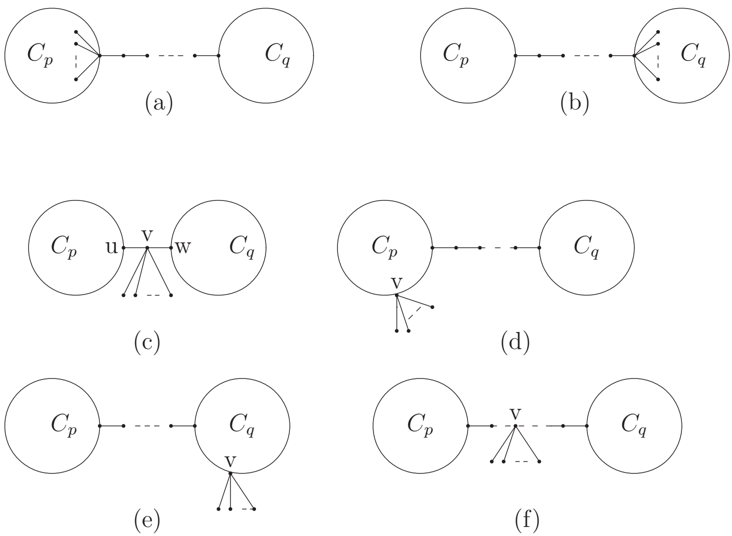


Figure 5. (a) $T_n^r(p, q)$; (b) $T_n^r(q, p)$; (c) $T_n(p, q)$.

Secondly, we find the bicyclic graph with the Zagreb indices in $\mathcal{B}(p, q)$.

Let $T_n^r(p,q)$ be the $(n,n+1)-$graph obtaining from connecting C_p and C_q by a path of length r and the other $n+1-p-q-r$ edges are all attached to the common vertex of the path and C_p, see Figure 5(a). $T_n^r(q,p)$ is showed in Figure 5(b). And $T_n(p,q)$ is the $(n,n+1)-$graph obtaining from connecting C_p and C_q by a path uvw of length 2 and the other $n-p-q-1$ edges are all attached to the vertex w of the path, as showed in Figure 5(c).

Theorem 3.7. If $G \in \mathcal{B}(p,q)$, the length of the shortest path connecting C_p and C_q in G is r, then either $(i=1,2)$

(i) $M_i(G) \le M_i(T_n^r(p,q))$ with the equality if and only if $G \cong T_n^r(p,q)$; or

(ii) $M_i(G) \le M_i(T_n^r(q,p))$ with the equality if and only if $G \cong T_n^r(q,p)$; or

(iii) $M_i(G) \le M_i(T_n(p,q))$ with the equality if and only if $G \cong T_n(p,q)$.

Proof. Let $W = v_1 v_2 \cdots v_r v_{r+1}$ be the shortest path connecting C_p and C_q in G, and v_1 the common vertex W and C_p, v_{r+1} the common vertex W and C_q.

Repeating the transformations A and B on graph G, we can get a graph G' in Figure 5 such that all the edges not on the cycles are the pendant edges attached to the same vertex v. By Lemmas 2.1 and 2.2, we have $M_i(G) \le M_i(G')$ $(i=1,2)$ with the equality if and only if all the edges not on the cycles are also the pendant edges attached to the same vertex in G.

Case I. v is on the cycle C_p, as showed in Figure 5(d).

$$\begin{aligned}
& M_1(T_n^r(p,q)) - M_1(G') \\
= \; & (n+4-p-q-r)^2 + 4 - (n+3-p-q-r)^2 - 9 \\
= \; & 2(n+1-p-q-r) \ge 0
\end{aligned}$$

with the equality if and only if $n = p+q+r-1$, and then also $G' \cong T_n^r(p,q)$.

(i) If v_1 and v are not adjacent, then

$$\begin{aligned}
& M_2(T_n^r(p,q)) - M_2(G') \\
= \; & (n+1-p-q-r)(n+4-p-q-r) + 4(n+4-p-q-r) \\
& +(n+4-p-q-r)d(v_2) + 8 - (n+1-p-q-r)(n+3-p-q-r) \\
& -4(n+3-p-q-r) - 3d(v_2) - 12 \\
= \; & (n+1-p-q-r)(1+d(v_2)) \ge 0
\end{aligned}$$

with the equality if and only if $n = p+q+r-1$, and then also $G' \cong T_n^r(p,q)$.

(ii) If v_1 and v are adjacent, then

$$\begin{aligned}
& M_2(T_n^r(p,q)) - M_2(G') \\
= \; & (n+1-p-q-r)(n+4-p-q-r) + 4(n+4-p-q-r) \\
& +(n+4-p-q-r)d(v_2) + 4 - (n+1-p-q-r)(n+3-p-q-r) \\
& -5(n+3-p-q-r) - 3d(v_2) - 6 \\
= \; & (n+1-p-q-r)d(v_2) \ge 0
\end{aligned}$$

with the equality if and only if $n = p+q+r-1$, and then also $G' \cong T_n^r(p,q)$.

Case II. v is on the cycle C_q, as showed in Figure 5(e). The proof is the same as in the case I.

Case III. v is on the path W, as showed in Figure 5(f). If $G' \ncong T_n(p,q)$, then $r \geq 3$. Let $v = v_t$, $1 < t \leq r$.

$$\begin{aligned} & M_1(T_n(p,q)) - M_1(G') \\ = & \ (n-1-p-q) + (n+1-p-q)^2 - (n+1-p-q-r) \\ & -(n+3-p-q-r)^2 - 2(r-2) \\ = & \ (r-2)(2n+3-2p-2q-r) \\ > & \ 0 \qquad\qquad\qquad (\text{since } n+1-p-q-r \geq 0 \text{ and } r > 3) \end{aligned}$$

If $2 < t < r$, then $r > 3$ and

$$\begin{aligned} & M_2(T_n(p,q)) - M_2(G') \\ = & \ (n-p-q-1)(n-p-q+1) + 6(n-p-q+1) \\ & -(n-p-q-r+1)(n-p-q-r+3) \\ & -4(n-p-q-r+3) - 4(r-4) - 12 \\ = & \ (r-1)(2n-2p-2q-r+3) - 3 \\ > & \ 0 \qquad\qquad (\text{since } n+1-p-q-r \geq 0 \text{ and } r > 3) \end{aligned}$$

If $t = 2$ or $t = r$, then

$$\begin{aligned} & M_2(T_n(p,q)) - M_2(G') \\ = & \ (n-p-q-1)(n-p-q+1) + 6(n-p-q+1) \\ & -(n-p-q-r+1)(n-p-q-r+3) - 5(n-p-q-r+3) \\ & -4(r-3) - 6 \\ = & \ (n-p-q)(2r-3) - (r-1)(r-3) + r - 4 \\ \geq & \ (r-1)(2r-3) - (r-1)(r-3) + r - 4 (\text{since } n+1-p-q-r \geq 0) \\ = & \ r^2 - 4 > 0 \end{aligned}$$

The proof is completed.

Lemma 3.8. $M_1(T_n(p,q)) \leq M_1(T_n(3,3))$ and $M_2(T_n(p,q)) \leq M_2(T_n(3,3))$ with the equality if and only if $p = q = 3$.

Proof. $M_1(T_n(p,q)) = (n+1-p-q)^2 + (n-1-p-q) + 18 + 4(p+q-2)$, $M_1(T_n(3,3)) = (n-5)^2 + (n-7) + 18 + 16$,

$$\begin{aligned} & M_1(T_n(3,3)) - M_1(T_n(p,q)) \\ = & \ (2n-p-q-4)(p+q-6) + (p+q-6) - 4(p+q-6) \\ = & \ (p+q-6)(2n-p-q-7) \\ \geq & \ (p+q-6)(n-6) \qquad\qquad (\text{since } n-p-q-1 \geq 0) \\ \geq & \ 0 \end{aligned}$$

with the equality if and only if $p+q = 6$, i.e., $p = q = 3$.

$M_2(T_n(p,q)) = (n+1-p-q)(n+5-p-q)+24+4(p+q-4),$
$M_2(T_n(3,3)) = (n-5)(n-1)+24+8,$

$$\begin{aligned} & M_2(T_n(3,3)) - M_2(T_n(p,q)) \\ = \ & (n-5)(n-1) - ((n-5)-(p+q-6))((n-1) \\ & -(p+q-6)) - 4(p+q-6) \\ = \ & (p+q-6)(2n-p-q-4) \\ \geq \ & (p+q-6)(n-3) \qquad \text{(since } n-p-q-1 \geq 0) \\ \geq \ & 0 \end{aligned}$$

with the equality if and only if $p+q=6$, i.e., $p=q=3$.

Lemma 3.9. If $r \geq 2$, then $M_i(T_n^r(p,q) < M_i(T_n^{r-1}(p,q))$, $i=1,2$.

Proof. By computing immediately, we have
$M_1(T_n^r(p,q)) = (n+1-p-q-r)+(n+4-p-q-r)^2+4(p+q+r-3)+9,$
$M_1(T_n^{r-1}(p,q)) = (n+2-p-q-r)+(n+5-p-q-r)^2+4(p+q+r-4)+9.$
And $M_1(T_n^{r-1}(p,q)) - M_1(T_n^r(p,q)) = 2(n+3-p-q-r) > 0.$
If $r > 2$, then
$M_2(T_n^r(p,q)) = (n+4-p-q-r)(n+7-p-q-r)+4(p+q+r-6)+18,$
$M_2(T_n^{r-1}(p,q)) = (n+5-p-q-r)(n+8-p-q-r)+4(p+q+r-7)+18.$
And $M_2(T_n^{r-1}(p,q)) - M_2(T_n^r(p,q)) = 2(n+4-p-q-r) > 0.$
If $r = 2$, then
$M_2(T_n^r(p,q)) = (n+2-p-q)(n+5-p-q)+4(p+q-4)+18,$
$M_2(T_n^{r-1}(p,q)) = (n+3-p-q)(n+7-p-q)+4(p+q-4)+12.$
And $M_2(T_n^{r-1}(p,q)) - M_2(T_n^r(p,q)) = 3(n+2-p-q) > 0.$

Lemma 3.10. $M_i(T_n^1(p,q)) \leq M_i(T_n^1(3,3))$, with the equality if and only if $p=q=3$, $i=1,2$.

Proof. By computing immediately, we have
$M_1(T_n^1(p,q)) = (n-p-q)+(n+3-p-q)^2+4(p+q-2)+9,$
$M_1(T_n^1(3,3)) = (n-6)+(n-3)^2+16+9.$

And $M_1(T_n^1(3,3)) - M_1(T_n^1(p,q)) = (p+q-6)(2n-3-p-q) \geq 0$ with the equality if and only if $p+q=6$, i.e., $p=q=3$.

$M_2(T_n^1(p,q)) = (n+3-p-q)(n+7-p-q)+4(p+q-4)+12,$
$M_2(T_n^1(3,3)) = (n-3)(n+1)+8+12.$

And $M_2(T_n^1(3,3)) - M_2(T_n^1(p,q)) = (p+q-6)(2n-p-q) \geq 0$ with the equality if and only if $p+q=6$, i.e., $p=q=3$.

Now, we compare the Zagreb indices of $T_n^1(3,3)$ and $T_n(3,3)$. It can be computed out easily that $M_i(T_n^1(3,3)) > M_i(T_n(3,3))$, $i=1,2$. So, we have

Theorem 3.11. The $T_n^1(3,3)$ is the unique graph with the largest Zagreb indices among all graphs in $\mathcal{B}(p,q)$ for all $p \geq 3$ and $q \geq 3$.

Thirdly, we find the bicyclic graph with the largest Zagreb indices in $\mathcal{C}(p,q,l)$.

Let $\theta_n^l(p,q)$ be the graph obtaining from the graph in Figure 1(c) by attaching $n+1+l-(p+q)$ to one of its vertices with degree 3 (see Figure 6(a)).

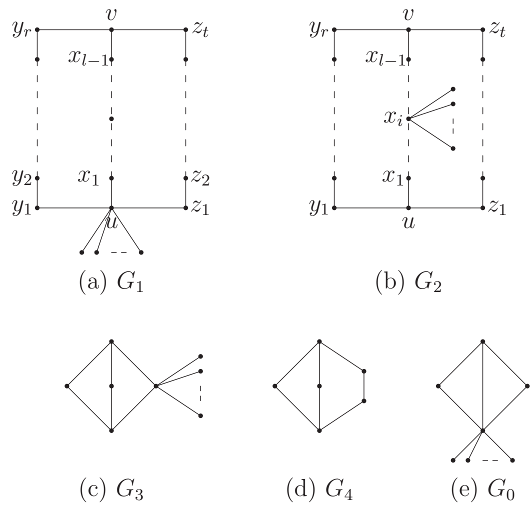


Figure 6. The graphs G_i, $i = 0,1,2,3,4$.

Theorem 3.12. Let $G \in \mathcal{C}(p,q,l)$. Then $M_i(G) \leq M_i(G_0)$ $(i = 1,2)$ with the equality if and only if $G \cong G_0$, where G_0 is the graph in Figure 6(e).

Proof. Repeating the transformations A and B on graph G, we can get a graph G' such that all the edges not on the cycles are the pendant edges attached to the same vertex v_0, i.e., G' is one of the graphs in Figure 6. By Lemmas 2.1 and 2.2, we have $M_i(G) \leq M_i(G')$ $(i = 1,2)$ with the equality if and only if all the edges not on the cycles are also the pendant edges attached to the same vertex in G.

Let $W_1 = ux_1x_2\cdots x_{l-1}v$ be the common path of C_p and C_q of the graph G' in Figure 6, $W_2 = uy_1y_2\cdots y_rv$ and $W_3 = uz_1z_2\cdots z_tv$ the other paths from u to v on C_p and C_q, respectively; $r = p-l-1$, $t = q-l-1$, $r \geq 0$, $t \geq 0$, $l \geq 1$ and $r+t+l \geq 3$.

By computing immediately, we have

$M_1(G_0) = (n-4)+(n-1)^2+17$,

$M_1(G_1) = (n-1-r-t-l)+(n+2-r-t-l)^2+4(r+t+l-1)+9$,

$M_1(G_2) = (n-1-r-t-l)+(n+1-r-t-l)^2+4(r+t+l-2)+18$,

$M_1(G_0)-M_1(G_1) = (r+t+l-3)(2n-2-r-t-l) \geq 0$ since $r+t+l \geq 3$

and $n-r-t-l-1 \geq 0$, with the equality if and only if $r+t+l=3$, i.e., $G' \cong G_0$;

$M_1(G_0) - M_1(G_2) = (r+t+l-3)(2n-3-r-t-l) + (n-r-t-l-1) + (n-4) \geq 0$ since $r+t+l \geq 3$ and $n-r-t-l-1 \geq 0$ and $n \geq 4$, with the equality if and only if $r+t+l=3$ and $n=4$, i.e., $G' \cong G_0$ (where $n=4$).

If there is an edge $e = xy$ in G_1 such that the degrees of x and y are equal two, then we can obtain a graph G_1' by contracting the edge e and attaching a pendant edge $e' = uu'$ to u, and we have $M_2(G_1') > M_2(G_1)$ since $d_{G_1}(x)d_{G_1}(y) = 4$ and $d_{G_1'}(u)d_{G_1'}(u') \geq 4$ and $d_{G_1}(u) < d_{G_1'}(u)$. So, $M_2(G_1) \geq M_2(G_0)$ with the equality if and only if $G_1 \cong G_0$.

If there are two edges e_1 and e_2 in G_2 such that the degrees of their end-vertices are equal two, then we can obtain a graph G_2' by contracting the edges e_1 and e_2 and attaching two pendant edges to x_i; or if there an edge e in G_2 such that the degrees of its end-vertices and e_2 are equal two, then we can obtain a graph G_2' by contracting the edge e and attaching a pendant edge to x_i. And we have $M_2(G_2') \geq M_2(G_2)$. So, $M_2(G_1) \geq M_2(G_3)$ or $M_2(G_2) \geq M_2(G_4)$.

It is computed out easily that $M_2(G_3) < M_2(G_0)$ and $M_2(G_4) < M_2(G_0)$. So, the proof is completed.

Finally, we give the bicyclic graphs with the largest Zagreb indice.

Theorem 3.13. G_0 is the unique graph with the the largest Zagreb indices M_1 and M_2 among all bicyclic graphs with n vertices.

Proof. From Theorem 3.6, Theorem 3.11 and Theorem 3.12, we only need to compare the Zagreb indices of $S_n(3,3)$, $T_n^1(3,3)$ and G_0. Computing immediately, we have

$M_1(T_n^1(3,3)) < M_1(S_n(3,3)) < M_1(G_0)$

$M_2(T_n^1(3,3)) < M_2(S_n(3,3)) < M_2(G_0)$

Therefore, G_0 has the largest Zagreb indices among all bicyclic graphs with n vertices.

It is surprising that the graphs with the largest Zagreb indices among the trees, unicyclic graphs and bicyclic graphs of order n are the same as those with the largest Merrifield-Simmons index [17,18,19] and the smallest Hosoya index [20,21].

4 Some transformations which decrease the Zagreb indices

In this section, we give two transformations which will decrease the Zagreb indices as follows:

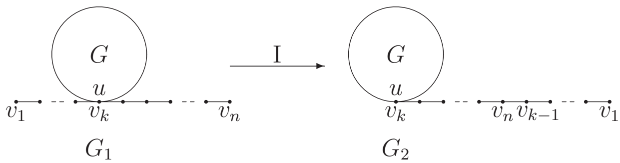


Figure 7. Transformation C.

Transformation C. Let $G \neq P_1$ be a connected graph and choose $u \in V(G)$. G_1 denotes the graph that results from identifying u with the vertex v_k of a simple path $v_1v_2\cdots v_n$, $1 < k < n$; G_2 is obtained from G_1 by deleting $v_{k-1}v_k$ and adding $v_{k-1}v_n$ (see Figure 7).

Lemma 4.1. Let G_1 and G_2 be the graphs in Figure 7. Then $M_i(G_1) > M_i(G_2)$, $i = 1, 2$.

Proof. By the definition of the Zagreb indices, we have

$$\begin{aligned} M_1(G_1) - M_1(G_2) &= (d_G(u)+2)^2 + 1 - (d_G(u)+1)^2 - 4 \\ &= 2d_G(u) > 0. \end{aligned}$$

$$\begin{aligned} & M_2(G_1) - M_2(G_2) \\ = \ & (d_G(u)+2)(\sum_{x \in N_G(u)} d_G(x) + d_{G_1}(v_{k-1}) + d_{G_1}(v_{k+1})) \\ & + d_{G_1}(v_{n-1})d_{G_1}(v_n) - (d_G(u)+1)(\sum_{x \in N_G(u)} d_G(x) + d_{G_2}(v_{k+1})) \\ & - d_{G_2}(v_{n-1})d_{G_2}(v_n) - d_{G_2}(v_n)d_{G_2}(v_{k-1}) \\ = \ & \begin{cases} \sum_{x \in N_G(u)} d_G(x), & \text{if } k = 2 \text{ and } n = 3; \\ \sum_{x \in N_G(u)} d_G(x) + d_G(u), & \text{if } k = 2 \text{ and } n > 3; \\ \sum_{x \in N_G(u)} d_G(x) + d_G(u), & \text{if } k > 2 \text{ and } n = k+1; \\ \sum_{x \in N_G(u)} d_G(x) + 2d_G(u), & \text{if } k > 2 \text{ and } n > k+1 \end{cases} \\ > \ & 0. \end{aligned}$$

Remark 3. Repeating Transformation C, any tree T attached to a graph G can be changed into a path as showed in Figure 8. And the Zagreb indices decrease.

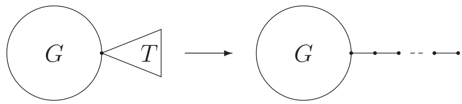


Figure 8.

Transformation D. Let u and v be two vertices in a graph G. G_1 denotes the graph that results from identifying u with the vertex u_0 of a path $u_0u_1u_2\cdots u_r$ and identifying v with the vertex v_0 of a path $v_0v_1v_2\cdots v_t$; G_2 is obtained from G_1 by deleting uu_1 and adding v_tu_1 (see Figure 9).

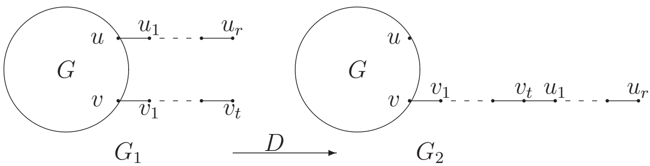


Figure 9. Transformation D.

Lemma 4.2. Let G_1 and G_2 be the graphs in Figure 9. $d_G(u) \geq d_G(v) > 1$, $r \geq 1$ and $t \geq 0$.

(i) If $t > 0$, then $M_1(G_1) > M_1(G_2)$ and $M_2(G_1) > M_2(G_2)$;

(ii) If $t = 0$ and $d_G(u) > d_G(v)$, then $M_1(G_1) > M_1(G_2)$;

(iii) If $t = 0$ and $\sum\limits_{x\in N_G(u)-\{v\}} d_G(x) > \sum\limits_{y\in N_G(v)-\{u\}} d_G(y)$, then $M_2(G_1) > M_2(G_2)$.

Proof. (i) Note that $d_G(u) > 1$ and $t > 0$, we have

$$\begin{aligned} M_1(G_1) - M_1(G_2) &= (d_{G_1}(u))^2 + (d_{G_1}(v_t))^2 - (d_{G_2}(u))^2 - (d_{G_2}(v_t))^2 \\ &= (d_G(u)+1)^2 + 1 - (d_G(u))^2 - 4 \\ &= 2d_G(u) - 2 > 0. \end{aligned}$$

$$\begin{aligned} & M_2(G_1) - M_2(G_2) \\ = \; & (d_G(u)+1)(\sum_{x\in N_G(u)} d_G(x) + d_{G_1}(u_1)) + d_{G_1}(v_{t-1})d_{G_1}(v_t) \\ & -d_G(u)\sum_{x\in N_G(u)} d_G(x) - d_{G_2}(v_{t-1})d_{G_2}(v_t) - d_{G_2}(v_t)d_{G_2}(u_1) \\ = \; & \begin{cases} \sum\limits_{x\in N_G(u)} d_G(x) + d_G(u) - d_G(v) - 2, & \text{if } r = 1 \text{ and } t = 1; \\ \sum\limits_{x\in N_G(u)} d_G(x) + d_G(u) - 3, & \text{if } r = 1 \text{ and } t > 1; \\ \sum\limits_{x\in N_G(u)} d_G(x) + 2d_G(u) - d_G(v) - 3, & \text{if } r > 1 \text{ and } t = 1; \\ \sum\limits_{x\in N_G(u)} d_G(x) + 2d_G(u) - 4, & \text{if } k > 1 \text{ and } t > 1 \end{cases} \\ > \; & 0. \end{aligned}$$

(ii) If $t = 0$ and $d_G(u) > d_G(v)$, then

$$\begin{aligned} M_1(G_1) - M_1(G_2) = &\ (d_{G_1}(u))^2 + (d_{G_1}(v_t))^2 - (d_{G_2}(u))^2 - (d_{G_2}(v_t))^2 \\ = &\ (d_G(u)+1)^2 + (d_G(v))^2 - (d_G(u))^2 - (d_G(v))^2 \\ = &\ 2d_G(u) - 2d_G(v) > 0. \end{aligned}$$

(iii) When u and v are not adjacent, we have

$$\begin{aligned} &M_2(G_1) - M_2(G_2) \\ =\ & (d_G(u)+1)(\sum_{x \in N_G(u)} d_G(x) + d_{G_1}(u_1)) + d_G(v) \sum_{y \in N_G(v)} d_G(y) \\ & - d_G(u) \sum_{x \in N_G(u)} d_G(x) - (d_G(v)+1)(\sum_{y \in N_G(v)} d_G(y) + d_{G_2}(u_1)) \\ =\ & \sum_{x \in N_G(u)} d_G(x) - \sum_{y \in N_G(v)} d_G(y) + d_{G_1}(u_1)(d_G(u) - d_G(v)) \\ & \qquad\qquad\qquad (\text{since } d_{G_1}(u_1) = d_{G_2}(u_1)) \\ >\ & 0. \end{aligned}$$

When u and v are adjacent, we have

$$\begin{aligned} &M_2(G_1) - M_2(G_2) \\ =\ & (d_G(u)+1)(\sum_{x \in N_G(u)-\{v\}} d_G(x) + d_{G_1}(u_1)) + d_G(v) \sum_{y \in N_G(v)-\{u\}} d_G(y) \\ & + (d_G(u)+1)d_G(v) - d_G(u) \sum_{x \in N_G(u)-\{v\}} d_G(x) \\ & - (d_G(v)+1)(\sum_{y \in N_G(v)-\{u\}} d_G(y) + d_{G_2}(u_1)) - d_G(u)(d_G(v)+1) \\ =\ & \sum_{x \in N_G(u)-\{v\}} d_G(x) - \sum_{y \in N_G(v)-\{u\}} d_G(y) + (d_{G_1}(u_1) - 1)(d_G(u) - d_G(v)) \\ & \qquad\qquad\qquad (\text{since } d_{G_1}(u_1) = d_{G_2}(u_1)) \\ >\ & 0. \end{aligned}$$

Remark 4. After repeating transformation C, if we repeat transformation D, then any tree can be changed into a path, any unicyclic graph can be changed into such an unicyclic graph that a path attached to a cycle, any bicyclic graph can be changed into such a bicyclic graph that a path attached to one of the graphs in Figure 10 (Lemma 4.2(i)). Moreover, the bicyclic graph can changed into such a bicyclic graph that the path is attached to a vertex of degree 2 (Lemma 4.2(ii)(iii)). And the Zagreb indices decrease.

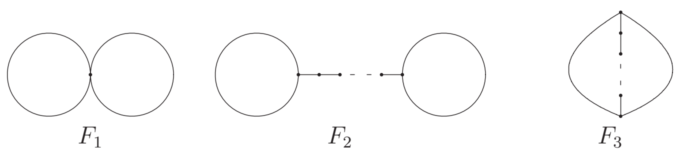


Figure 10.

Lemma 4.3. If there is a path $x_1x_2 \cdots x_k$ $(k > 1)$ attached to the vertex x_1 in G_1, then $M_i(G_1) > M_i(G_2)$, $i = 1, 2$, where G_2 is obtained from G_1 by deleting x_1v and adding x_kv, as showed in Figure 11.

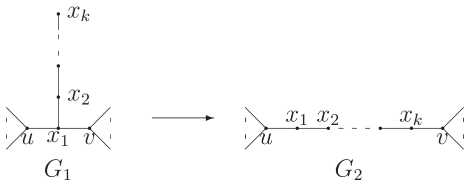


Figure 11.

Proof. Note that only the degrees of x_1 and x_k are changed, we have

$$M_1(G_1) - M_1(G_2) = 9 + 1 - 4 - 4 > 0.$$

If $k > 2$, then

$$M_2(G_1) - M_2(G_2) = d(u) + d(v) > 0.$$

If $k = 2$, then

$$M_2(G_1) - M_2(G_2) = d(u) + d(v) - 1 > 0.$$

So, $M_i(G_1) > M_i(G_2)$, $i = 1, 2$.

5 The smallest Zagreb indices among all the trees, unicyclic graphs and bicyclic graphs

In this section, we characterize the tree, the unicyclic graph and the bicyclic graph with the smallest Zagreb index.

From Lemma 4.1, we have

Theorem 5.1([4,7]). Let T be any tree of order n. If T is different from P_n, then $M_1(T) > M_1(P_n)$ and $M_2(T) > M_2(P_n)$.

Let F_n^k be the unicyclic graph obtained by attaching a path of length $n - k$ to the cycle C_k of length k. From Lemmas 4.1 and 4.2, we have

Theorem 5.2. Let G be an unicyclic graph of order n and girth k. If G is different from F_n^k, then $M_1(G) > M_1(F_n^k)$ and $M_2(G) > M_2(F_n^k)$.

Using Lemma 4.3, we have

Theorem 5.3([9,15]). The cycle C_n is the unique graph with the smallest Zagreb indices M_1 and M_2 among all unicyclic graphs with n vertices.

Let F_1, F_2 and F_3 be the bicyclic graphs with n vertices showed in Figure 10. From Remark 4 (or Lemma 4.2) and Lemma 4.3, we know that the bicyclic graph with the smallest Zagreb index is one of the graphs F_1, F_2 and F_3. And

$M_1(F_1) = 4n + 12,$
$M_1(F_2) = M_1(F_3) = 4n + 10;$
$M_2(F_1) = 4n + 20,$
$M_2(F_2) = M_2(F_3) =$

$$\begin{cases} 4n+16, & \text{if two vertices with degree 3 are adjacent;} \\ 4n+17, & \text{if two vertices with degree 3 are not adjacent} \end{cases}$$

So, we have

Theorem 5.4. The bicyclic graphs of order n with the smallest Zagreb indices are the graphs F_2 and F_3 in which the vertices of degree 3 are not adjacent except $n = 4, 6$.

Finally, we survey some results on the extremal graphs for the Zagreb indices, the Hosoya index and the Merrifield-Simmons index in trees, unicyclic graphs and $(n, n+1)$-graphs from [4,7,9,15-26], respectively.

Zagreb indices	largest	smallest
trees of order n	S_n	P_n
uncyclic graphs of order n	$S_n + e$	C_n
$(n, n+1)$-graphs	F_0	F_2 or F_3

Hosoya index	largest	smallest
trees of order n	P_n	S_n
unicyclic graphs of order n	C_n	$S_n + e$
$(n, n+1)$-graphs	H_0 or $K_{2,3}$	F_0

Merrifield-Simmons index	largest	smallest
trees of order n	S_n	P_n
uncyclic graphs of order n	$S_n + e$ or C_4	C_n
$(n, n+1)$-graphs	F_0	H_0 or $K_{2,3}$

where F_0 is obtained from S_n by adding two adjacent edges, H_0 is the graph connecting two cycle C_3s by a path of length $n - 5$.

Remark 5. The author know that the minimum M_1 when the numbers of vertices and edges are given was obtained by Prof. I. Gutman [27] from the the referee, also the smallest M_1 for trees, unicyclic graphs, bicyclic graphs and more are known. The author would like to thank the referee for valuable suggestions.

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