

Comparing the Zagreb indices for connected bicyclic graphs ^{*†}

Lingli Sun[‡]

*Department of Maths and Informatics Sciences, College of Sciences
Huazhong Agricultural University, Wuhan, 430070, P.R.China*

Shouliu Wei

*Department of Mathematics
Minjiang University, Fuzhou, 350108, P.R.China*

(Received October 6, 2008)

Abstract

The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of a (molecule) graph G are defined as $M_1(G) = \sum_{u \in V(G)} (d(u))^2$ and $M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$, where $d(u)$ denotes the degree of a vertex u in G . The AutoGraphiX system [1] [4] [5] conjectured $M_1/n \leq M_2/m$ (where $n = |V(G)|$ and $m = |E(G)|$) for simple connected graphs. Hansen and Vukičević [11] proved it is true for chemical graphs and it does not hold for all general graphs. Vukičević and Graovac [22] proved that it is also true for trees. Liu [15] proved that it is true for unicyclic graphs. In this paper, we show that $M_1/n \leq M_2/m$ holds for connected bicyclic graphs except one class and characterize the extremal graph. Additionally, we construct the counterexamples of connected bicyclic graphs from the the class we exclude.

*The project was supported financially by the fund of Huazhong Agricultural University.

†This paper is dedicated to Professor Jingzhong Mao on the occasion of his 70th birthday.

‡Corresponding author. E-mail: sunlingli@yahoo.com.cn

1 Introduction

For a molecular graph G , the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined in [10] as

$$M_1(G) = \sum_{u \in V(G)} (d(u))^2, \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v),$$

where $d(u)$ denotes the degree of the vertex u of G . The research background of Zagreb index together with its generalization appears in chemistry or mathematical chemistry. The readers are referred to literatures [2] [8] [9] [13] [14] [19] [21] and the references therein.

A natural issue is to compare the values of the Zagreb indices on the same graph. Observe that, for general graphs, the order of magnitude of M_1 is $O(n^3)$ (n vertices and degrees in $O(n)$, squared) while the order of magnitude of M_2 is $O(n^4)$ ($m = O(n^2)$ edges and degrees in $O(n)$, squared). This suggests comparing M_1/n with M_2/m instead of M_1 and M_2 .

Use of the AutoGraphiX system [1] [4] [5] led to the following conjecture:

Conjecture 1.1 *For all simple connected graphs G :*

$$M_1(G)/n \leq M_2(G)/m$$

and the bound is tight for complete graphs.

Hansen and Vukičević [11] proved it is true for chemical graphs and it does not hold for all general graphs. Vukičević and Graovac [22] proved that it is also true for trees. Liu [15] proved that it is true for unicyclic graphs. In this paper, we show that it holds for connected bicyclic graphs except one class and characterize the extremal graph. Additionally, we construct the counterexamples of connected bicyclic graphs from the the class we exclude.

First we introduce some graph notations used in this paper. We only consider finite, undirected and simple graphs. If $xy \in E(G)$, we say that y is a *neighbor* of x and denote by $N_G(x)$ the set of neighbors of x . Denote $N_G[x] = N_G(x) \cup \{x\}$. $d_G(x) = |N_G(x)|$ is called the *degree* of x . A *pendant vertex* is a vertex with degree one. A *hook* is the unique neighbor of a pendant vertex. We denote the set of hooks of G by $H(G)$.

A closed trail whose origin and internal vertices are distinct is a *cycle*. A cycle of length k is called a k -*cycle*, denoted by C_k . A *bipartite graph* is one whose vertex set can be partitioned into two subsets X and Y , so that each edge has one end in X and one end in Y ; such a partition (X, Y) is called *bipartition* of the graph. A *complete bipartite graph* is a simple bipartite graph with bipartition (X, Y) in which each vertex of X is joined to each vertex of Y ; if $|X| = m$ and $|Y| = n$, such a graph is denoted by $K_{m,n}$.

Suppose that V' is a nonempty subset of $V(G)$. The subgraph of G whose vertex is V' and whose edge set is the set of those edges of G that have both ends in V' is called the subgraph of G *induced* by V' and is denoted by $G[V']$.

We denote the number of vertices of degree i in G by n_i and the number of edges that connect vertices of degree i and j by m_{ij} , where we do not distinguish m_{ij} and m_{ji} .

2 Comparing the Zagreb indices for connected bicyclic graphs without pendant vertices

If G is a connected bicyclic graph without pendant vertices, then G belongs to one of the three cases in Fig. 1. It is clear that G is a chemical graph in any case. Although Hansen and Vukičević [11] proved $M_1(G)/n \leq M_2(G)/m$ is true for chemical graphs, to complete the proof of our main theorem, we give a simple proof.

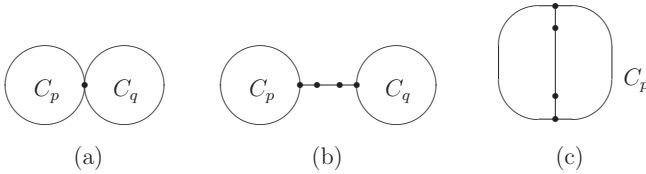


Figure 1

We compute and compare the Zagreb indices in three cases:

Case (a) It is easy to have $n_2 = n - 1$, $n_4 = 1$, $m_{22} = n + 1 - 4 = n - 3$ and $m_{24} = 4$. Therefore, we have $M_1(G) = 4(n - 1) + 16 = 4n + 12$ and $M_2(G) = 4(n - 3) + 32 = 4n + 20$. Since $n \geq 5$, we have $M_1(G)/n < M_2(G)/m$.

Case (b) It is easy to have $n_2 = n - 2$ and $n_3 = 2$. Therefore, we have $M_1(G) = 4(n - 2) + 18 = 4n + 10$.

Subcase 1 If $m_{33} = 1$, we have $m_{22} = n - 4$ and $m_{23} = 4$. Then $M_2(G) = 4(n - 4) + 24 + 9 = 4n + 17$.

Subcase 2 Otherwise $m_{33} = 0$. We have $m_{22} = n + 1 - 6 = n - 5$ and $m_{23} = 6$. Then $M_2(G) = 4(n - 5) + 36 = 4n + 16$.

Since $n \geq 6$, we have $M_1(G)/n < M_2(G)/m$ in both subcases.

Case (c) Similar to case (b), we have $M_1(G) = 4n + 10$, $M_2(G) = 4n + 17$ if $m_{33} = 1$ and $M_2(G) = 4n + 16$ if $m_{33} = 0$.

If $m_{33} = 1$, since $n \geq 4$, we have $M_1(G)/n < M_2(G)/m$.

If $m_{33} = 0$, since $n \geq 5$, we have $M_1(G)/n \leq M_2(G)/m$, with the equality holds if and only if $n = 5$, i.e., $G = K_{2,3}$.

In summary, we have the following theorem:

Theorem 2.1 *If G is a connected bicyclic graph without pendant vertices, then*

$$M_1(G)/n \leq M_2(G)/m,$$

with the equality holds if and only if $G = K_{2,3}$.

3 Comparing the Zagreb indices for connected bicyclic graphs

Let G be a connected bicyclic graph with pendant vertices. For any vertex $u \in H(G)$, $N_G(u) = \{v_1, v_2, \dots, v_k\}$ ($k \geq 2$). Denote $\mathbb{A} = \{G : d_G(v_1) = 2, d_G(v_i) = 1, i = 2, 3, \dots, k\}$

Lemma 3.1 *If $G \notin \mathbb{A}$ is a connected bicyclic graph with pendant vertices, then there exists a subgraph F such that $G - F$ is a connected bicyclic graph and $G - F \notin \mathbb{A}$.*

Proof. If there exists a vertex $u \in H(G)$ such that u is adjacent to at least two pendant vertices, let v be a pendant vertex adjacent to u . We are easy to see that $G - v$ is a connected bicyclic graph and $G - v \notin \mathbb{A}$.

Now we may assume that each vertex in $H(G)$ is adjacent to unique pendant vertex.

If there exists a pendant vertex w such that $G - w \notin \mathbb{A}$, let $F = w$. Then $G - F$ is a connected bicyclic graph and $G - F \notin \mathbb{A}$.

Otherwise for each pendant vertex x , we have $G - x \in \mathbb{A}$. Then G contains the structure in Fig. 2, in which $d(u_i) = 2, i = 0, 2, 3, \dots, t, d(u_1) = 3, d(u_{t+1}) \geq 3$ ($t \geq 2$) and $d(v_j) = 1, j = 0, 1$.

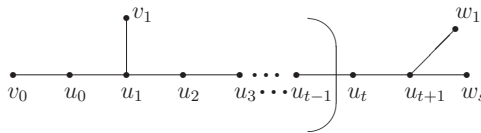


Figure 2

Let $N(u_{t+1}) = \{u_t, w_1, w_2, \dots, w_s\}$ ($s \geq 2$), then we have $d(w_i) \geq 2, i = 1, 2, \dots, s$. Otherwise if there exists w_1 such that $d(w_1) = 1$, then w_1 is the unique pendant vertex adjacent to u_{t+1} . If $s \geq 3$, then $G - w_1 \notin \mathbb{A}$, a contradiction. If $s = 2$, since G is a connected bicyclic graph, all the neighbors of w_s except u_{t+1} can't be pendant vertices. Then $G - w_1 \notin \mathbb{A}$, a contradiction.

Let $F = G[\{v_0, v_1, u_0, u_1, u_2, \dots, u_{t-1}\}]$ ($t \geq 2$). Then $G - F$ is a connected bicyclic graph and $G - F \notin \mathbb{A}$. □

Remark: From the proof of lemma 3.1, we are easy to see that F is either a pendant vertex or a subgraph with at least four vertices.

Theorem 3.2 *If $G \notin \mathbb{A}$ is a connected bicyclic graph with n vertices and m edges, then*

$$M_1(G)/n \leq M_2(G)/m,$$

with the equality holds if and only if $G = K_{2,3}$.

Proof. If G is a connected bicyclic graph without pendant vertices, by theorem 2.1, we have $M_1(G)/n \leq M_2(G)/m$, with the equality holds if and only if $G = K_{2,3}$. So we may assume that G is a connected bicyclic graph with pendant vertices in the following proof.

Since G is a connected bicyclic graph, we have $m = n + 1$. We prove by induction on n . If $n = 5$, then $G = G_1$ or G_2 (see Fig.3) and we are easy to have $M_1(G_1)/n = \frac{32}{5} < M_2(G_1)/m = \frac{42}{6}$ and $M_1(G_2)/n = \frac{34}{5} < M_2(G_2)/m = \frac{44}{6}$. Thus the result is true.

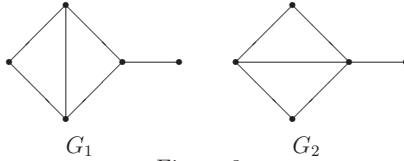


Figure 3

Suppose that it holds for all connected bicyclic graphs except \mathbb{A} with vertices less than n (having pendant vertices).

By Lemma 3.1, we have that there exists a subgraph F such that $G - F$ is a connected bicyclic graph and $G - F \notin \mathbb{A}$. We choose F such that $|F|$ is as small as possible. By the proof of Lemma 3.1, we have that F is either a pendant vertex or a subgraph with at least four vertices. Thus we divide our proof into two cases:

Case 1. F is a pendant vertex.

Let $v = F$ and u be its unique neighbor and $N_G(u) = \{v, v_1, v_2, \dots, v_k\}$ ($k \geq 1$).

Let $G' = G - v$. Then G' is a connected bicyclic graph with $n - 1$ vertices and $G' \notin \mathbb{A}$. By the induction hypothesis, we have

$$\frac{M_1(G')}{n - 1} \leq \frac{M_2(G')}{n},$$

which implies $M_1(G') < M_2(G')$.

Furthermore, we have

$$M_1(G) = M_1(G') + 2k + 2,$$

$$M_2(G) = M_2(G') + \sum_{i=1}^k d_G(v_i) + k + 1.$$

Since G is a connected bicyclic graph and $G \notin \mathbb{A}$, we have $\sum_{i=1}^k d_G(v_i) \geq k + 2$.

So we divide our proof into two cases:

Case 1.1 $\sum_{i=1}^k d_G(v_i) \geq k + 3$.

Then $\sum_{i=1}^k d_G(v_i) + k + 1 \geq 2k + 4$. So we have

$$\begin{aligned} nM_2(G) &= n(M_2(G') + \sum_{i=1}^k d_G(v_i) + k + 1) \\ &\geq nM_2(G') + n(2k + 4) \\ &= (n - 1)M_2(G') + M_2(G') + 2kn + 2n + 2n \\ &> nM_1(G') + M_1(G') + 2kn + 2n + (2k + 2) \\ &= (n + 1)M_1(G') + (2k + 2)(n + 1) \\ &= (n + 1)M_1(G), \end{aligned}$$

which implies $M_1(G)/n < M_2(G)/m$.

Case 1.2 $\sum_{i=1}^k d_G(v_i) = k + 2$.

Subcase 1 $d_G(v_k) = 3$ and $d_G(v_i) = 1, i = 1, 2, \dots, k - 1$.

(a) $k \geq 2$.

Claim 1. $M_2(G') - M_1(G') > k - 1$.

Proof. Let $N(v_k) = \{u, w_1, w_2\}$. Since G is a connected bicyclic graph, there exists $d_G(w_2) \geq 2$.

If $d_G(w_2) \geq 3$ or $d_G(w_1) \geq 2$, let $\tilde{G} = G' - \bigcup_{i=1}^{k-1} \{v_i\}$. Then \tilde{G} is a connected bicyclic graph and $\tilde{G} \notin \mathbb{A}$. By the induction hypothesis, we have

$$\frac{M_1(\tilde{G})}{n - k} \leq \frac{M_2(\tilde{G})}{n - k + 1},$$

which implies $M_1(\tilde{G}) < M_2(\tilde{G})$.

Furthermore, we have

$$\begin{aligned} M_1(G') &= M_1(\tilde{G}) + k^2 - 1 + k - 1, \\ M_2(G') &= M_2(\tilde{G}) + 3(k - 1) + k(k - 1), \\ M_2(G') - M_1(G') &> k - 1. \end{aligned}$$

Otherwise $d_G(w_1) = 1$ and $d_G(w_2) = 2$. Let $N(w_2) = \{v_k, w_3\}$. Since G is a connected bicyclic graph, we have $d_G(w_3) \geq 2$.

If $d_G(w_3) \geq 3$, let $G_1 = G' - \{w_1, u\} \cup \bigcup_{i=1}^{k-1} \{v_i\}$. Then G_1 is a connected bicyclic graph and $G_1 \notin \mathbb{A}$. By the induction hypothesis, we have

$$\frac{M_1(G_1)}{n - k - 2} \leq \frac{M_2(G_1)}{n - k - 1},$$

which implies $M_1(G_1) < M_2(G_1)$.

Furthermore, we have

$$M_1(G') = M_1(G_1) + k^2 + k + 8,$$

$$M_2(G') = M_2(G_1) + k^2 + 2k + 7,$$

$$M_2(G') - M_1(G') > k - 1.$$

Otherwise $d_G(w_3) = 2$. We continue to consider the neighbor of w_3 until we find a path $w_2 w_3 \cdots w_s$ such that $d_G(w_s) \geq 3$ ($s \geq 4$). Let $G_2 = G' - \{u, w_1\} \cup \bigcup_{i=1}^k \{v_i\} \cup \bigcup_{j=2}^{s-3} \{w_j\}$ ($G_2 = G' - \{u, w_1\} \cup \bigcup_{i=1}^k \{v_i\}$ if $s = 4$). Then G_2 is a connected bicyclic graph and $G_2 \notin \mathbb{A}$. By the induction hypothesis, we have

$$\frac{M_1(G_2)}{n - k - s + 1} \leq \frac{M_2(G_2)}{n - k - s + 2},$$

which implies $M_1(G_2) < M_2(G_2)$.

Furthermore, we have

$$M_1(G') = M_1(G_2) + k^2 + k + 4s - 4,$$

$$M_2(G') = M_2(G_2) + k^2 + 2k + 4s - 5,$$

$$M_2(G') - M_1(G') > k - 1.$$

This completes the proof of claim 1. □

By claim 1, we have

$$\begin{aligned} nM_2(G) &= n(M_2(G')) + \sum_{i=1}^k d_G(v_i) + k + 1 \\ &= nM_2(G') + n(2k + 3) \\ &= (n - 1)M_2(G') + M_2(G') + 2kn + 2n + n \\ &> nM_1(G') + M_1(G') + k - 1 + 2kn + 2n + (k + 3) \\ &= (n + 1)M_1(G') + (2k + 2)(n + 1) \\ &= (n + 1)M_1(G), \end{aligned}$$

which implies $M_1(G)/n < M_2(G)/m$.

(b) $k = 1$.

Then from above, we have

$$M_1(G) = M_1(G') + 4, \quad M_2(G) = M_2(G') + 5.$$

$$\begin{aligned} nM_2(G) &= n(M_2(G') + 5) \\ &= nM_2(G') + 5n \\ &= (n-1)M_2(G') + M_2(G') + 5n \\ &> nM_1(G') + M_1(G') + 5n \\ &> (n+1)M_1(G') + 4(n+1) \\ &= (n+1)M_1(G), \end{aligned}$$

which implies $M_1(G)/n < M_2(G)/m$.

Subcase 2 $d_G(v_k) = d_G(v_{k-1}) = 2$ and $d_G(v_i) = 1, i = 1, 2, \dots, k-2$.

(a) $k \geq 3$.

Claim 2. $M_2(G') - M_1(G') > k - 2$.

Proof. Let $N(v_k) = \{u, w\}$ and $N(v_{k-1}) = \{u, w'\}$. Since G is a connected bicyclic graph, without loss of generality, we may assume $d_G(w) \geq 2$.

If $d(w') \geq 2$, let $\bar{G} = G' - \bigcup_{i=1}^{k-2} \{v_i\}$. Then \bar{G} is a connected bicyclic graph and $\bar{G} \notin \mathbb{A}$. By the induction hypothesis, we have

$$\frac{M_1(\bar{G})}{n-k+1} \leq \frac{M_2(\bar{G})}{n-k+2},$$

which implies $M_1(\bar{G}) < M_2(\bar{G})$.

Furthermore, we have

$$\begin{aligned} M_1(G') &= M_1(\bar{G}) + k^2 - 4 + k - 2, \\ M_2(G') &= M_2(\bar{G}) + 4(k-2) + k(k-2), \\ M_2(G') - M_1(G') &> k - 2. \end{aligned}$$

Otherwise $d_G(w') = 1$.

If $d_G(w) \geq 3$, let $G_3 = G' - \{w'\} \cup \bigcup_{i=1}^{k-1} \{v_i\}$. Then G_3 is a connected bicyclic graph and $G_3 \notin \mathbb{A}$. By the induction hypothesis, we have

$$\frac{M_1(G_3)}{n-k-1} \leq \frac{M_2(G_3)}{n-k},$$

which implies $M_1(G_3) < M_2(G_3)$.

Furthermore, we have

$$M_1(G') = M_1(G_3) + k^2 + k + 2,$$

$$M_2(G') = M_2(G_3) + k^2 + 2k,$$

$$M_2(G') - M_1(G') > k - 2.$$

Otherwise $d_G(w) = 2$. We continue to consider the neighbor of w until we find a path $w_1(=w)w_2 \cdots w_p$ such that $d_G(w_p) \geq 3$ ($p \geq 2$). Let $G_4 = G' - \{u, w'\} \cup \bigcup_{i=1}^k \{v_i\} \cup \bigcup_{j=1}^{p-3} \{w_j\}$ ($G_4 = G' - \{u, w'\} \cup \bigcup_{i=1}^{k-1} \{v_i\}$ if $p = 2$, $G_4 = G' - \{u, w'\} \cup \bigcup_{i=1}^k \{v_i\}$ if $p = 3$). Then G_4 is a connected bicyclic graph and $G_4 \notin \mathbb{A}$. By the induction hypothesis, we have

$$\frac{M_1(G_4)}{n - k - p} \leq \frac{M_2(G_4)}{n - k - p + 1},$$

which implies $M_1(G_4) < M_2(G_4)$.

Furthermore, we have

$$M_1(G') = M_1(G_4) + k^2 + k + 4p - 2,$$

$$M_2(G') = M_2(G_4) + k^2 + 2k + 4p - 4,$$

$$M_2(G') - M_1(G') > k - 2.$$

This completes the proof of claim 2. □

By claim 2, we have

$$\begin{aligned} nM_2(G) &= n(M_2(G') + \sum_{i=1}^k d_G(v_i) + k + 1) \\ &= nM_2(G') + n(2k + 3) \\ &= (n - 1)M_2(G') + M_2(G') + 2kn + 2n + n \\ &> nM_1(G') + M_1(G') + k - 2 + 2kn + 2n + (k + 4) \\ &= (n + 1)M_1(G') + (2k + 2)(n + 1) \\ &= (n + 1)M_1(G), \end{aligned}$$

which implies $M_1(G)/n < M_2(G)/m$.

(b) $k = 2$.

Then from above, we have

$$M_1(G) = M_1(G') + 6, \quad M_2(G) = M_2(G') + 7.$$

$$\begin{aligned}
 nM_2(G) &= n(M_2(G') + 7) \\
 &= nM_2(G') + 7n \\
 &= (n - 1)M_2(G') + M_2(G') + 7n \\
 &> nM_1(G') + M_1(G') + 7n \\
 &> (n + 1)M_1(G') + 6(n + 1) \\
 &= (n + 1)M_1(G),
 \end{aligned}$$

which implies $M_1(G)/n < M_2(G)/m$.

Case 2. F is a subgraph with at least four vertices.

Note that in this case, since we choose F such that $|F|$ is as small as possible, we have the following results:

- (1) Each vertex in $H(G)$ is adjacent to unique pendant vertex;
- (2) For each pendant vertex x , $G - x \in \mathbb{A}$.

By the proof of lemma 3.1, let $F = G[\{v_0, v_1, u_0, u_1, u_2, \dots, u_{t-1}\}]$, in which $d(u_i) = 2$, $i = 0, 2, 3, \dots, t$, $d(u_1) = 3$, $d(u_{t+1}) \geq 3$ ($t \geq 2$) and $d(v_j) = 1$, $j = 0, 1$.

Let $\widehat{G} = G - F$. By lemma 3.1, we have that \widehat{G} is a connected bicyclic graph and $\widehat{G} \notin \mathbb{A}$. By induction hypothesis, we have

$$\frac{M_1(\widehat{G})}{n - t - 2} \leq \frac{M_2(\widehat{G})}{n - t - 1},$$

which implies $M_1(\widehat{G}) < M_2(\widehat{G})$.

Furthermore, we have

$$M_1(G) = M_1(\widehat{G}) + 4t + 10,$$

$$M_2(G) = M_2(\widehat{G}) + d_G(u_{t+1}) + 4t + 9.$$

Case 2.1 $d_G(u_{t+1}) \geq 5$.

Then we have

$$\begin{aligned}
 nM_2(G) &= n(M_2(\widehat{G}) + d_G(u_{t+1}) + 4t + 9) \\
 &\geq nM_2(\widehat{G}) + n(4t + 14) \\
 &= (n - t - 2)M_2(\widehat{G}) + (t + 2)M_2(\widehat{G}) + 4tn + 14n \\
 &> (n - t - 1)M_1(\widehat{G}) + (t + 2)M_1(\widehat{G}) + 4tn + 14n \\
 &= (n + 1)M_1(\widehat{G}) + 4tn + 14n \\
 &> (n + 1)M_1(\widehat{G}) + (n + 1)(4t + 10) \\
 &= (n + 1)M_1(G),
 \end{aligned}$$

which implies $M_1(G)/n < M_2(G)/m$.

Case 2.2 $d_G(u_{t+1}) = 4$.

Let $N(u_{t+1}) = \{u_t, w_1, w_2, w_3\}$. By the proof of lemma 3.1, we have $d(w_i) \geq 2$, $i = 1, 2, 3$.

Let $G^* = \widehat{G} - u_t$. Then G^* is a connected bicyclic graph and $G^* \notin \mathbb{A}$. By the induction hypothesis, we have

$$\frac{M_1(G^*)}{n-t-3} \leq \frac{M_2(G^*)}{n-t-2},$$

which implies $M_1(G^*) < M_2(G^*)$.

Furthermore, we have

$$M_1(\widehat{G}) = M_1(G^*) + 16 - 9 + 1,$$

$$M_2(\widehat{G}) = M_2(G^*) + \sum_{i=1}^3 d_G(w_i) + 4,$$

$$\begin{aligned} M_2(\widehat{G}) - M_1(\widehat{G}) &= M_2(G^*) + \sum_{i=1}^3 d_G(w_i) + 4 - [M_1(G^*) + 16 - 9 + 1] \\ &\geq M_2(G^*) - M_1(G^*) + 10 - 8 \\ &> 2. \end{aligned}$$

So we have

$$\begin{aligned} nM_2(G) &= n(M_2(\widehat{G}) + 4t + 13) \\ &= (n-t-2)M_2(\widehat{G}) + (t+2)M_2(\widehat{G}) + 4tn + 13n \\ &> (n-t-1)M_1(\widehat{G}) + (t+2)M_1(\widehat{G}) + 2(t+2) + 4tn + 13n \\ &= (n+1)M_1(\widehat{G}) + 4tn + 13n + 2t + 4 \\ &> (n+1)M_1(\widehat{G}) + (n+1)(4t+10) \\ &= (n+1)M_1(G), \end{aligned}$$

which implies $M_1(G)/n < M_2(G)/m$.

Case 2.3 $d_G(u_{t+1}) = 3$.

Claim 3. $M_2(\widehat{G}) \geq M_1(\widehat{G}) + 2$.

Let $N(u_{t+1}) = \{u_t, w_1, w_2\}$. By the proof of lemma 3.1, we have $d(w_i) \geq 2$, $i = 1, 2$. Since G is a connected bicyclic graph, there exists $z \in N(w_2)$ such that $d_G(z) \geq 2$.

If $d_G(w_1) \geq 3$, let $G^0 = \widehat{G} - u_t$. Then G^0 is a connected bicyclic graph and $G^0 \notin \mathbb{A}$. By the induction hypothesis, we have

$$\frac{M_1(G^0)}{n-t-3} \leq \frac{M_2(G^0)}{n-t-2},$$

which implies $M_1(G^0) < M_2(G^0)$.

Furthermore, we have

$$M_1(\widehat{G}) = M_1(G^0) + 9 - 4 + 1,$$

$$M_2(\widehat{G}) = M_2(G^0) + \sum_{i=1}^2 d_G(w_i) + 3,$$

$$\begin{aligned} M_2(\widehat{G}) - M_1(\widehat{G}) &= M_2(G^0) + \sum_{i=1}^2 d_G(w_i) + 3 - [M_1(G^0) + 9 - 4 + 1] \\ &\geq M_2(G^0) - M_1(G^0) + 8 - 6 \\ &> 2. \end{aligned}$$

Otherwise $d_G(w_1) = 2$. Let $N(w_1) = \{u_{t+1}, y\}$. Then we have $d_G(y) \geq 2$. Otherwise if $d_G(y) = 1$, then $G - y \notin \mathbb{A}$, a contradiction.

If $d_G(w_2) \geq 3$, let $G^1 = \widehat{G} - u_t$. Then G^1 is a connected bicyclic graph and $G^1 \notin \mathbb{A}$. By the induction hypothesis, we have

$$\frac{M_1(G^1)}{n-t-3} \leq \frac{M_2(G^1)}{n-t-2},$$

which implies $M_1(G^1) < M_2(G^1)$.

Furthermore, we have

$$M_1(\widehat{G}) = M_1(G^1) + 9 - 4 + 1,$$

$$M_2(\widehat{G}) = M_2(G^1) + \sum_{i=1}^2 d_G(w_i) + 3,$$

$$\begin{aligned} M_2(\widehat{G}) - M_1(\widehat{G}) &= M_2(G^1) + \sum_{i=1}^2 d_G(w_i) + 3 - [M_1(G^1) + 9 - 4 + 1] \\ &\geq M_2(G^1) - M_1(G^1) + 8 - 6 \\ &> 2. \end{aligned}$$

Otherwise $d_G(w_2) = 2$ and $N(w_2) = \{u_{t+1}, z\}$, $d_G(z) \geq 2$. let $G^2 = \widehat{G} - u_t$. Then G^2 is a connected bicyclic graph and $G^2 \notin \mathbb{A}$. By the induction hypothesis, we have

$$\frac{M_1(G^2)}{n-t-3} \leq \frac{M_2(G^2)}{n-t-2},$$

which implies $M_1(G^2) < M_2(G^2)$. Since $M_1(G^2)$ and $M_2(G^2)$ are integers, we have $M_1(G^2) + 1 \leq M_2(G^2)$.

Furthermore, we have

$$\begin{aligned}
 M_1(\widehat{G}) &= M_1(G^2) + 9 - 4 + 1, \\
 M_2(\widehat{G}) &= M_2(G^2) + \sum_{i=1}^2 d_G(w_i) + 3, \\
 M_2(\widehat{G}) - M_1(\widehat{G}) &= M_2(G^2) + \sum_{i=1}^2 d_G(w_i) + 3 - [M_1(G^2) + 9 - 4 + 1] \\
 &= M_2(G^2) - M_1(G^2) + 7 - 6 \\
 &\geq 2.
 \end{aligned}$$

This completes the proof of claim 3. □

By claim 3, we have

$$\begin{aligned}
 nM_2(G) &= n(M_2(\widehat{G}) + 4t + 12) \\
 &= (n - t - 2)M_2(\widehat{G}) + (t + 2)M_2(\widehat{G}) + 4tn + 12n \\
 &\geq (n - t - 1)M_1(\widehat{G}) + (t + 2)M_1(\widehat{G}) + 2(t + 2) + 4tn + 12n \\
 &= (n + 1)M_1(\widehat{G}) + 4tn + 12n + 2t + 4 \\
 &> (n + 1)M_1(\widehat{G}) + (n + 1)(4t + 10) \\
 &= (n + 1)M_1(G),
 \end{aligned}$$

which implies $M_1(G)/n < M_2(G)/m$.

This completes the proof of the theorem. □

4 The counterexamples of connected bicyclic graphs for $M_1(G)/n \leq M_2(G)/m$

In section 3, we exclude one class of connected bicyclic graphs for there exist the counterexamples (see Fig.3).

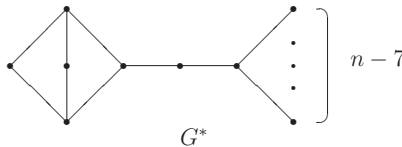


Figure 3

We may assume $n(G^*) \geq 18$. Now we compute the Zagreb indices of G^* . We have $n_1 = n - 7$, $n_2 = 3$, $n_3 = 3$, $n_{n-6} = 1$, $m_{23} = 5$, $m_{33} = 2$, $m_{1(n-6)} = n - 7$ and $m_{2(n-6)} = 1$. Therefore, we have $M_1(G) = n - 7 + 12 + 27 + (n - 6)^2 = n^2 - 11n + 68$ and $M_2(G) = 30 + 18 + (n - 6)(n - 7) + 2(n - 6) = n^2 - 11n + 78$. Since $n \geq 18$, we have $M_1(G)/n > M_2(G)/m$.

Acknowledgement. The authors would like to thank anonymous referees for their valuable comments.

References

- [1] M. Aouchiche, J.M. Bonnefoy, A. Fidahoussen, G. Caporossi, P. Hansen, L. Hiesse, J. Lacheré and A. Monhait, *Variable Neighborhood Search for Extremal Graphs*. 14. *The AutoGraphiX 2 system*, in: L. Liberti and N. Maculan (Eds.), *Global Optimization: From Theory to Implementation*, Springer, 2005.
- [2] A. T. Balaban, I. Motoc, D. Bonchev and O. Mekenyan, Topological indices for structure–activity correlations, *Topics Curr. Chem.* **114** (1983) 21–55.
- [3] J. A. Bonday and U. S. Murty, *Graph Theory and Its Applications*, MacMillan, London, 1976.
- [4] G. Caporossi and P. Hansen, Variable neighborhood search for extremal graphs: 1 The AutoGraphiX system, *Discr. Math.* **212** (2000) 29-44.
- [5] G. Caporossi and P. Hansen, Variable neighborhood search for extremal graphs. 5. Three ways to automate finding conjectures, *Discr. Math.* **276** (2004) 81-94.
- [6] K. C. Das and I. Gutman, Some properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 103–112.
- [7] H. Deng, A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 597–616.
- [8] I. Gutman and K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.
- [9] I. Gutman, B. Rušćić and C. F. Wilcox, Graph theory and molecular orbitals. 12. Acyclic polyenes, *J. Chem. Phys.* **62** (1975) 3399–3405.

- [10] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. Total π -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.
- [11] P. Hansen and D. Vukičević, Comparing the Zagreb indices, *Croat. Chem. Acta*, **80** (2007) 165–168.
- [12] Y. Hou and J. Li, Bounds on the largest eigenvalues of trees with a given size of matching, *Lin. Algebra Appl.* **342** (2002) 203–217.
- [13] L. B. Kier and L. H. Hall, *Molecular Connectivity in Chemistry and Drug Research*, Academic Press, San Francisco, 1976.
- [14] L. B. Kier and L. H. Hall, *Molecular Connectivity in Structure–Activity Analysis*, Wiley, New York, 1986.
- [15] B. Liu, On a conjecture about comparing Zagreb indices, *Recent Results in the Theory of Randić Index* (Mathematical Chemistry Monographs 6), Univ. Kragujevac, Kragujevac, 2008, 205–209.
- [16] B. Liu and I. Gutman, Upper bounds for Zagreb indices of connected graphs, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 439–446.
- [17] B. Liu and I. Gutman, Estimating the Zagreb and the general Randić indices, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 617–632.
- [18] H. Liu, M. Lu and F. Tian, Trees of extremal connectivity index, *Discr. Appl. Math.* **154** (2006) 106–119.
- [19] S. Nikolić, G. Kovačević, A. Miličević and N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta* **76** (2003) 113–124.
- [20] X. F. Pan, H. Q. Liu and J. M. Xu, Sharp lower bounds for the general Randić index of trees with a given size of matching, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 465–480.
- [21] R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.
- [22] D. Vukičević and A. Graovac, Comparing Zagreb M_1 and M_2 indices for acyclic molecules, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 587–590.

- [23] Z. Yan, H. Liu and H. Liu, Sharp bounds for the second Zagreb index of unicyclic graphs, *J. Math. Chem.*, **42** (2007) 565–574.
- [24] H. Zhang and S. Zhang, Unicyclic graphs with the first three smallest and largest first general Zagreb index, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 427–438.
- [25] B. Zhou, Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 113–118.
- [26] B. Zhou, Remarks on Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 591–596.
- [27] B. Zhou and I. Gutman, Further properties of Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 233–239.