

Some Extremal Results for Vertex–Degree–Based Invariants

Yuedan Yao^a, Muhuo Liu^{a,b,*}, Kinkar Ch. Das^c, Yingshi Ye^a

^a*Department of Mathematics, South China Agricultural University,
Guangzhou, 510642, China*

^b*College of Mathematics and Statistics, Shenzhen University,
Shenzhen, 518060, China*

^c*Department of Mathematics, Sungkyunkwan University,
Suwon 440-746, Republic of Korea
kinkardas2003@googlemail.com*

(Received February 5, 2018)

Abstract

For a symmetric bivariable function $f(x, y)$, let the connectivity function of a connected graph G be $M_f(G) = \sum_{uv \in E(G)} f(d(u), d(v))$, where $d(u)$ is the degree of vertex u . As an application of majorization theory, we present a uniform method to some extremal results together with its corresponding extremal graphs for vertex-degree-based invariants among the class of trees, unicyclic graphs and bicyclic graphs with fixed number of independence number and/or matching number, respectively. As a consequence, several known results in chemical graph theory has been obtained.

1 Introduction

In this paper, we only consider simple connected undirected graph, and $G = (V, E)$ is a connected graph with n vertices and m edges. If $m = n + c - 1$, then G is called a c -cyclic graph. Especially, when $c = 0, 1$ or 2 , then G is called a *tree*, *unicyclic graph* or *bicyclic graph*, respectively. As usual, denote $d(u)$ the degree of u . A vertex of degree one is called a *pendent vertex* of G , and the number of pendent vertices of G will be referred as $p(G)$. In contrast with pendent vertex, a vertex of degree being at least two is called

*Corresponding author (liumuhuo@163.com)

a *non-pendent vertex*. Furthermore, a vertex with degree k will be referred as a k -vertex. Suppose the degree of vertex v_i equals d_i for $i = 1, 2, \dots, n$, then $\pi(G) = (d_1, d_2, \dots, d_n)$ is called the *degree sequence* of G . In the following discussions we enumerate the degrees in non-increasing order, i.e., $d_1 \geq d_2 \geq \dots \geq d_n$. Consequently, $d(v_1) \geq d(v_2) \geq \dots \geq d(v_n)$ holds, where $V(G) = \{v_1, v_2, \dots, v_n\}$. Let $\Gamma(\pi)$ be the class of connected graphs with degree sequence π . When G is a c -cyclic graph with degree sequence π , then

$$\sum_{i=1}^n d_i = 2(n + c - 1). \tag{1}$$

A subset S of $V(G)$ is said to be an *independent set* of G if each pair of vertices of S are not adjacent. The number of vertices in a maximum independent set of G is called the *independence number* of G and denoted by $\alpha(G)$. If G is a connected graph with $n \geq 3$ vertices, then it is easy to see that the class of pendent vertices form an independent vertex set of G . Thus, we have

$$p(G) \leq \alpha(G). \tag{2}$$

A *matching* in a graph G is a set of pairwise nonadjacent edges. The maximum size of a matching set of G is called the *matching number* of G and denoted by $\beta(G)$ hereafter. For any connected graph G , since each edge of any matching has at least one end vertex being a non-pendent vertex, we have

$$p(G) \leq n - \beta(G). \tag{3}$$

Among all the vertex-degree-based graph invariants, the *first Zagreb index* $M_1(G)$ and *second Zagreb index* $M_2(G)$ [2] are two famous topological indices, where

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

In what follows, γ denotes a real number. As a generalization of $M_1(G)$, Li and Zheng [4] introduced the notation of *general Randić index* $R_\gamma(G)$ (sometimes also referred as “zeroth-order general Randić index”), where

$$R_\gamma(G) = \sum_{v \in V(G)} (d(v))^\gamma.$$

Furthermore, $R_{-1}(G)$ is called the *inverse degree* of graph G and denoted by $ID(G)$ (See [12]).

Since $\sum_{uv \in E(G)} (d(u) + d(v)) = \sum_{v \in V(G)} (d(v))^2$, as another extension to $M_1(G)$, the *general sum-connectivity index* [14] $\chi_\gamma(G)$ of G is constructed as

$$\chi_\gamma(G) = \sum_{uv \in E(G)} (d(u) + d(v))^\gamma.$$

The *reformulated Zagreb index* $Z_2(G)$ of G [9] is a slight modification to $\chi_2(G)$, where

$$Z_2(G) = \sum_{uv \in E(G)} (d(u) + d(v) - 2)^2.$$

As an extension of $Z_2(G)$, we define $Z_\gamma(G)$ as follows:

$$Z_\gamma(G) = \sum_{uv \in E(G)} (d(u) + d(v) - 2)^\gamma.$$

In order to study on vertex-degree-based invariants of a graph, Wang [10] recently proposed the concept of *escalating function* as follows: A symmetric bivariate function $f(x, y)$ defined on positive real numbers is called *escalating* if

$$f(x_1, x_2) + f(y_1, y_2) \geq f(x_2, y_1) + f(x_1, y_2) \tag{4}$$

holds for any $x_1 \geq y_1 > 0$ and $x_2 \geq y_2 > 0$, and the inequality in (4) is strict if $x_1 > y_1$ and $x_2 > y_2$. Furthermore, an escalating function $f(x, y)$ is called *good escalating* if $f(x, y)$ satisfies

$$\frac{\partial f(x, y)}{\partial x} > 0, \quad \frac{\partial^2 f(x, y)}{\partial x^2} \geq 0,$$

and

$$f(x_1 + 1, x_2) + f(x_1 + 1, y_1 - 1) \geq f(x_2, y_1) + f(x_1, y_1)$$

holds for any $x_1 \geq y_1$ and $x_2 \geq 1$. To extend these above definitions of vertex-degree-based invariants, Wang [10] defined *connectivity function* of a connected graph G associated with a symmetric bivariate function $f(x, y)$ as

$$M_f(G) = \sum_{uv \in E(G)} f(d(u), d(v)). \tag{5}$$

In this paper, we will employ the majorization theorem as a tool to give a uniform method for some extremal results together with its corresponding extremal graphs of vertex-degree-based invariants among the class of trees, unicyclic graphs and bicyclic graphs with fixed number of independence number and/or matching number, respectively.

2 Some useful preliminaries

As stated in [6, 13], the majorization theorem is an important and effective tool to deal with extremal problem of graph spectrum and topological index theory. In this section, we shall introduce some majorization theorems for vertex-degree-based invariants. Firstly, we introduce the definition of *majorization*.

Definition 2.1 (See [6, 8]) Let $\pi = (a_1, a_2, \dots, a_n)$ and $\pi' = (a'_1, a'_2, \dots, a'_n)$ be two different non-increasing sequences of nonnegative real numbers, we write $\pi \trianglelefteq \pi'$ if and only if $\sum_{i=1}^n a_i = \sum_{i=1}^n a'_i$, and $\sum_{i=1}^j a_i \leq \sum_{i=1}^j a'_i$ for all $j = 1, 2, \dots, n$. Furthermore, we write $\pi \triangleleft \pi'$ if and only if $\pi \trianglelefteq \pi'$ and $\pi \neq \pi'$. The ordering $\pi \trianglelefteq \pi'$ is sometimes called *majorization*.

A real valued function $f(x)$ defined on a convex set D is said to be strictly convex if

$$f(\lambda x + (1 - \lambda)y) < \lambda f(x) + (1 - \lambda)f(y)$$

holds for all $0 \leq \lambda \leq 1$ and all $x, y \in D$. The following majorization theorem for a strictly convex function had been discovered long time ago [3].

Theorem 2.1 [3] *Let $\pi = (a_1, a_2, \dots, a_n)$ and $\pi' = (b_1, b_2, \dots, b_n)$ be two non-increasing sequences of nonnegative real numbers. If $\pi \triangleleft \pi'$ and φ is a strictly convex function, then $\sum_{i=1}^n \varphi(a_i) < \sum_{i=1}^n \varphi(b_i)$.*

Note that $\varphi(x) = x^r$ is a strictly convex function for either $r > 1$ or $r < 0$, and $\varphi(x) = -x^r$ is a strictly convex function for $0 < r < 1$. Thus, Theorem 2.1 implies the following corollary.

Corollary 2.1 *Let $\pi = (a_1, a_2, \dots, a_n)$ and $\pi' = (b_1, b_2, \dots, b_n)$ be two non-increasing sequences of nonnegative real numbers. If $\pi \triangleleft \pi'$, then $\sum_{i=1}^n a_i^r < \sum_{i=1}^n b_i^r$ holds for either $r > 1$ or $r < 0$, and $\sum_{i=1}^n a_i^r > \sum_{i=1}^n b_i^r$ holds for $0 < r < 1$.*

For a given degree sequence π and a good escalating function $f(x, y)$, if G has the maximum connectivity function in $\Gamma(\pi)$, then G is called an *extremal graph* of $\Gamma(\pi)$.

Theorem 2.2 *Let π and π' be two different non-increasing degree sequences with $\pi \triangleleft \pi'$.*

(i) [5] *If $G \in \Gamma(\pi)$ and $G' \in \Gamma(\pi')$, then $R_\gamma(G) < R_\gamma(G')$ holds for either $\gamma < 0$ or $\gamma > 1$, and $R_\gamma(G) > R_\gamma(G')$ holds for $0 < \gamma < 1$.*

(ii) [7] *Let G and G' be an extremal c -cyclic graph of $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. If $f(x, y)$ is a good escalating function, then $M_f(G) < M_f(G')$ holds for $c \in \{0, 1, 2\}$.*

Theorem 2.3 [7] *The second Zagreb index $M_2(G)$ is good escalating, $Z_\gamma(G)$ and $\chi_\gamma(G)$ are also good escalating for $\gamma > 1$.*

3 Extremal results with given independence number

Denote by $\mathcal{R}(G)$ the reduced graph obtained from G by recursively deleting pendent vertices of the resultant graph until no pendent vertices remain. If G is a c -cyclic graph with $c \geq 1$, it is easy to see that $\mathcal{R}(G)$ is unique and $\mathcal{R}(G)$ is also a c -cyclic graph. Hereafter, let $\pi_1 = (2c + p, 2^{(n-p-1)}, 1^{(p)})$, $\pi_2 = (2c + p - 2, 3^{(2)}, 2^{(n-p-3)}, 1^{(p)})$ and $\pi_3 = (2c + p - 4, 4, 3^{(2)}, 2^{(n-p-4)}, 1^{(p)})$.

Lemma 3.1 *Let G be a c -cyclic graph with n vertices, p pendent vertices and degree sequence π . If $\pi \neq \pi_1$, then $\pi \triangleleft \pi_1$. Furthermore, $(2c + p, 2^{(n-p-1)}, 1^{(p)}) \triangleleft (2c + p + 1, 2^{(n-p-2)}, 1^{(p+1)})$.*

Proof. By Definition 2.1, it is easy to check that $(2c + p, 2^{(n-p-1)}, 1^{(p)}) \triangleleft (2c + p + 1, 2^{(n-p-2)}, 1^{(p+1)})$. Now, we turn to prove $\pi \triangleleft \pi_1$. To do this, let $\pi_1 = (d'_1, d'_2, \dots, d'_{n-p}, 1^{(p)})$ and $\pi = (d_1, d_2, \dots, d_{n-p}, 1^{(p)})$, where $d_1 \geq d_2 \geq \dots \geq d_{n-p} \geq 2$. Then,

$$d_1 = 2(n + c - 1) - p - d_2 - d_3 - \dots - d_{n-p} \leq 2(n + c - 1) - p - 2(n - p - 1) = 2c + p.$$

If $d_1 = 2c + p$, then $d_2 = d_3 = \dots = d_{n-p} = 2$, and hence $\pi = \pi_1$, a contradiction. Thus, $d_1 < 2c + p$. Since $d_j \geq 2$ holds for $2 \leq j \leq n - p$,

$$\sum_{i=1}^j d_i = 2(n + c - 1) - p - d_{j+1} - \dots - d_{n-p} \leq 2(n + c - 1) - p - 2(n - p - j) = \sum_{i=1}^j d'_i$$

holds for $2 \leq j \leq n - p$. Thus, $\pi \triangleleft \pi_1$. ■

As usual, let P_n , C_n and K_n be the path, cycle and complete graph with n vertices, respectively. An s -rose graph is a graph with exactly s cycles that all meet in one vertex.

Lemma 3.2 *Let G be a c -cyclic graph with n vertices, p pendent vertices and degree sequence π such that every vertex of $\mathcal{R}(G)$ is adjacent to at least one pendent vertex.*

(i) *If $\pi \neq \pi_2$ and $c \geq 1$, then $\pi \triangleleft \pi_2$. (ii) If $\pi \neq \pi_3$ and $c \geq 2$, then $\pi \triangleleft \pi_3$.*

Proof. Let $\pi(G) = (d_1, d_2, \dots, d_{n-p}, 1^{(p)})$, where $d_1 \geq d_2 \geq \dots \geq d_{n-p} \geq 2$. Since $c \geq 1$, G contains at least one cycle such that every vertex of this cycle is adjacent to at least one pendent vertex. Thus, we have $d_1 \geq d_2 \geq d_3 \geq 3$ and hence $\pi \triangleleft \pi_2$ by (1). So, (i) holds.

Now, we turn to prove (ii). Since $c \geq 2$, we may suppose that C_s and C_t are two cycles of G . Thus, each vertex of C_s and C_t is adjacent to at least one pendent vertex, and hence the degree of every vertex on C_s or C_t is at least three. Furthermore, since G is connected, there is at least one vertex with degree being at least four. In this case, we may suppose that $\pi = (d_1, d_2, \dots, d_{n-p}, 1^{(p)})$, where $d_1 \geq d_2 \geq \dots \geq d_k \geq 4 > d_{k+1} = d_{k+2} = \dots = d_q = 3 > d_{q+1} = d_{q+2} = \dots = d_{n-p} = 2$. By the former argument, $k \geq 1$ and $q \geq 4$.

If $k = 1$, then $\mathcal{R}(G)$ is a c -rose graph (since every vertex of $\mathcal{R}(G)$ is adjacent to at least one pendent vertex). Thus, $\pi = (d_1, 3^{(q-1)}, 2^{(n-p-q)}, 1^{(p)})$ and $q \geq s + t - 1 \geq 5$. In this case,

$$d_1 = 2(n + c - 1) - p - 3(q - 1) - 2(n - p - q) = 2c + p - q + 1 \leq 2c + p - 4$$

$$\text{and } d_1 + d_2 = 2(n + c - 1) - p - 3(q - 2) - 2(n - p - q) = 2c + 4 + p - q < 2c + p.$$

Now, it is easy to check that $\pi \triangleleft \pi_3$, as $d_3 \geq d_4 \geq 3$. Otherwise, $k \geq 2$. In this case, $\pi(B) = (d_1, d_2, \dots, d_k, 3^{(q-k)}, 2^{(n-p-q)}, 1^{(p)})$. Since $q \geq 4$, $k \geq 2$ and $\pi \neq \pi_3$, we have $\pi \triangleleft \pi_3$. ■

Lemma 3.3 *Let G be a c -cyclic graph with n vertices and degree sequence $\pi = (d_1, d_2, \dots, d_{n-p}, 1^{(p)})$ such that $d_3 \geq 3$. If $\pi \neq \pi_2$ and $c \geq 2$, then $\pi \triangleleft \pi_2$.*

Proof. We may suppose that $d_1 \geq d_2 \geq \dots \geq d_q \geq 3 > d_{q+1} = d_{q+2} = \dots = d_{n-p} = 2$. Since $d_3 \geq 3$, we have $q \geq 3$ and hence

$$\pi \triangleleft (2c + 1 + p - q, 3^{(q-1)}, 2^{(n-p-q)}, 1^{(p)}) \triangleleft \pi_2.$$

This completes the proof of this result. ■

Let v be a vertex of a graph G . Suppose $P_s = u_1 u_2 \dots u_s$, where $u_i \notin V(G)$ for $1 \leq i \leq s$. If we obtain G' by identifying the vertex v with u_1 , then we say that G' is obtained from G by *attaching the path P_s to v of G* . As shown in Figure 1, let F_1 and F_2 be two c -cyclic graphs, where $c \geq 1$. Hereafter, let $S_1(c; a, b)$ (resp., $S_2(c; a, b)$) define the c -cyclic graph obtained by attaching a paths of lengths two and b paths of lengths one, respectively, to the vertex v of F_1 (resp., F_2). If $c = 0$, then we agree with $a + b \geq 2$ and we define $S_1(0; a, b)$ as the tree obtained by attaching a paths of lengths two and b paths of lengths one, respectively, to one common vertex.

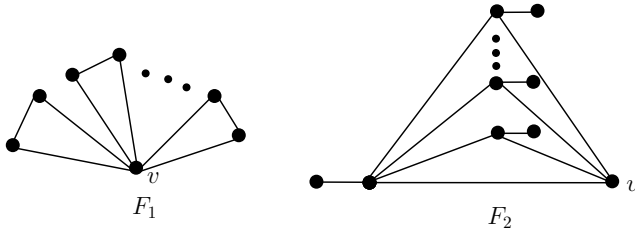


Figure 1. The c -cyclic graphs F_1 and F_2 .

In what follows, let $\pi_4 = (2c + a + b, 2^{(a+2c)}, 1^{(a+b)})$ and $\pi_5 = (c + 1 + a + b, c + 2, 3^{(c)}, 2^{(a)}, 1^{(a+b+c+1)})$. It is easy to see that $S_1(c; a, b) \in \Gamma(\pi_4)$ and $S_2(c; a, b) \in \Gamma(\pi_5)$.

Lemma 3.4 *Let G be a c -cyclic graph such that $G \in \Gamma(\pi_4)$, where $c \geq 0$ and $2c + a + b \geq 2$. If exactly $2c$ vertices of degrees two are not adjacent to any pendent vertex in G , then $G \cong S_1(c; a, b)$.*

Proof. We may suppose that $c \geq 1$, as the case of $c = 0$ can be proved similarly. Since G is a c -cyclic graph with $d_2 = 2$, $\mathcal{R}(G)$ is just a c -rose graph. Thus, each vertex of $V(\mathcal{R}(G)) \setminus \{v_1\}$ is not adjacent to any pendent vertex. Since exactly $2c$ vertices of degrees two of G are not adjacent to any pendent vertex, we can conclude that each cycle of G is a triangle, and hence each vertex of $V(G) \setminus V(\mathcal{R}(G))$ is adjacent to at least one pendent vertex.

Let u be a 2-vertex of G such that $u \notin V(\mathcal{R}(G))$. Since u is adjacent to at least one pendent vertex, we can conclude that u is adjacent to exactly one pendent vertex (Otherwise, G is disconnected, a contradiction). If u is adjacent to another 2-vertex (say v), then v is adjacent to a pendent vertex and u , which implies that G is disconnected, a contradiction. Thus, u is adjacent to one pendent vertex and the maximum degree vertex. Now, we can conclude that $G \cong S_1(c; a, b)$. ■

Lemma 3.5 *Let G be a c -cyclic graph such that $G \in \Gamma(\pi_5)$, where $c \geq 1$ and $a + b \geq 1$. If every non-pendent vertex of G is adjacent to at least one pendent vertex, then $G \cong S_2(c; a, b)$.*

Proof. Since every non-pendent vertex of G is adjacent to at least one pendent vertex and $G \in \Gamma(\pi_5)$, then the degree of each vertex of $V(\mathcal{R}(G))$ is at least three. By the definition of π_5 , $\mathcal{R}(G)$ is a c -cyclic graph with at most $c + 2$ vertices and the third maximum degree vertex of $\mathcal{R}(G)$ is a 2-vertex. Thus, $\mathcal{R}(G) \cong \mathcal{R}(F_2)$.

Since every non-pendent vertex of G is adjacent to at least one pendent vertex, similar with the proof of Lemma 3.4, we can conclude that every 2-vertex of G is adjacent to one pendent vertex and the maximum degree vertex. Now, we can conclude that $G \cong S_2(c; a, b)$. ■

Let $B_1(a, b)$ be the bicyclic graph obtained from $S_1(1; a, b)$ by adding one edge between two 2-vertices in $V(S_1(1; a, b)) \setminus V(C_3)$, where $a \geq 2$ and let $B_2(a, b)$ be the bicyclic graph obtained from $S_1(1; a, b)$ by adding one edge between one 2-vertex of $V(C_3)$ and one 2-vertex of $V(S_1(1; a, b)) \setminus V(C_3)$, where $a \geq 1$. In what follows, let $\pi_6 = (a + b + 2, 3^{(2)}, 2^{(a)}, 1^{(a+b)})$ and let $K_4 - e$ be a bicyclic graph obtained by deleting one edge from K_4 .

Lemma 3.6 *Let B be a bicyclic graph such that $B \in \Gamma(\pi_6)$, where $a + b \geq 1$. If all the non-pendent vertices being not adjacent to any pendent vertex induce either K_2 or K_3 , then either $B \cong B_1(a, b)$ or $B \cong B_2(a, b)$.*

Proof. Suppose that C_s and C_t are two cycles of B with $t \geq s \geq 3$, and suppose that $\pi_6 = (d_1, d_2, \dots, d_n)$. Since except for at most three non-pendent vertices, each of the other non-pendent vertices of B is adjacent to at least one pendent vertex, there are at least $|V(C_s \cup C_t)| - 3$ vertices with degree being at least three. Note that $d_2 = 3$ and $d_4 = 2$. Thus, $4 \leq |V(C_s) \cup V(C_t)| \leq 6$ and $1 \leq |V(C_s) \cap V(C_t)| \leq 3$.

We firstly consider the case of $|V(C_s) \cap V(C_t)| = 1$. Note that all the non-pendent vertices being not adjacent to any pendent vertex induce either K_2 or K_3 . Combining this with $d_2 = 3$ and $d_4 = 2$, we have $|V(C_s) \cup V(C_t)| = 5$ and $s = t = 3$. By the hypothesis, v_2 and v_3 are two adjacent 3-vertices in the same triangle of B , and v_2 and v_3 are adjacent to exactly one pendent vertex, respectively. Furthermore, the other two adjacent 2-vertices in the same triangle of B are not adjacent to any pendent vertex. Let u be a 2-vertex of B such that $u \notin V(\mathcal{R}(B))$. Then, u is adjacent to at least one pendent vertex. Since B is connected, u is adjacent to one pendent vertex and the maximum degree vertex. Now, we can conclude that $B \cong B_1(a, b)$ with $a \geq 2$.

We secondly consider the case of $|V(C_s) \cap V(C_t)| = 2$. In this case, we have $(s, t) \in \{(3, 3), (3, 4), (3, 5), (4, 4)\}$. Note that all the non-pendent vertices being not adjacent to any pendent vertex induce either K_2 or K_3 . Combining this with $d_2 = 3$ and $d_4 = 2$, we have $\mathcal{R}(B) \cong K_4 - e$. Now, since $d_2 = 3$ and $d_4 = 2$, one 3-vertex and one 2-vertex of $K_4 - e$ cannot be adjacent to any pendent vertex. Since B is connected, each of the other

2-vertices not in $K_4 - e$ is adjacent with exactly one pendent vertex and the maximum degree vertex. Now, by the definition of B and π_6 , we have $B \cong B_2(a, b)$ with $a \geq 1$.

We thirdly consider the case of $|V(C_s) \cap V(C_t)| = 3$. In this case, $(s, t) \in \{(4, 4), (4, 5)\}$. Note that all the non-pendent vertices being not adjacent to any pendent vertex induce either K_2 or K_3 . Thus, we have $d_4 \geq 3$, a contradiction. ■

For convenience, we rewrite $S_1(0; n - 1 - \alpha, 2\alpha + 1 - n)$ as $T(n, \alpha)$, $S_1(1; n - \alpha - 2, 2\alpha + 1 - n)$ as $U_1(n, \alpha)$, $S_2(1; n - \alpha - 3, 2\alpha + 1 - n)$ as $U_2(n, \alpha)$, $B_1(n - \alpha - 2, 2\alpha + 1 - n)$ as $Z_1(n, \alpha)$, $B_2(n - \alpha - 2, 2\alpha + 1 - n)$ as $Z_2(n, \alpha)$, $S_1(2; n - \alpha - 3, 2\alpha + 1 - n)$ as $Z_3(n, \alpha)$, and rewrite $S_2(2; n - \alpha - 4, 2\alpha + 1 - n)$ as $Z_4(n, \alpha)$.

Theorem 3.1 *Let T be a tree with $n (\geq 3)$ vertices and independence number α . If $T \not\cong T(n, \alpha)$, then (i) $R_\gamma(T) < R_\gamma(T(n, \alpha))$ holds for either $\gamma < 0$ or $\gamma > 1$, and $R_\gamma(T) > R_\gamma(T(n, \alpha))$ holds for $0 < \gamma < 1$, and (ii) $M_f(T) < M_f(T(n, \alpha))$ holds for any good escalating function $f(x, y)$.*

Proof. Since T is a bipartite graph, we have $\alpha \geq \lceil \frac{n}{2} \rceil$. We suppose that T contains p pendent vertices and suppose the degree sequence of T is π . By (2) and since $n \geq 3$, we have $2 \leq p \leq \alpha$. Let $\pi' = (\alpha, 2^{(n-\alpha-1)}, 1^{(\alpha)})$.

Suppose that $T \in \Gamma(\pi')$. Since $p = \alpha$, the class of pendent vertices of T form a maximum independent vertex set of T , and hence every non-pendent vertex must be adjacent to at least one pendent vertex. By Lemma 3.4, we have $T \cong T(n, \alpha)$, and hence

$$\Gamma(\pi') = \{T(n, \alpha)\}. \tag{6}$$

By (6), we have $\pi \neq \pi'$.

If $p = \alpha$ and $\pi \neq \pi'$, then $\pi \triangleleft \pi'$ by Lemma 3.1.

Otherwise, $p \leq \alpha - 1$. In this case, Lemma 3.1 implies that $\pi \triangleleft (\alpha - 1, 2^{(n-\alpha)}, 1^{(\alpha-1)}) \triangleleft \pi'$.

In both cases, the results follow from Theorem 2.2 and (6). ■

Corollary 3.1 *Let T be a tree with $n (\geq 3)$ vertices and independence number α . If $T \not\cong T(n, \alpha)$, then (i) [11] $\chi_\gamma(T) < \chi_\gamma(T(n, \alpha))$ holds for $\gamma \geq 1$, (ii) [1] $M_1(T) < M_1(T(n, \alpha))$ and $M_2(T) < M_2(T(n, \alpha))$, and (iii) [12] $ID(T) < ID(T(n, \alpha))$.*

Proof. By Theorems 2.3 and 3.1, the results hold. ■

Theorem 3.2 *Let U be a unicyclic graph with n vertices and independence number α , where $3 \leq \alpha \leq n - 3$. If $U \notin \{U_1(n, \alpha), U_2(n, \alpha)\}$, then (i) $R_\gamma(U) < \max \{R_\gamma(U_1(n, \alpha)),$*

$R_\gamma(U_2(n, \alpha))\}$ for $\gamma < 0$ or $\gamma > 1$ and $R_\gamma(U) > \min \{R_\gamma(U_1(n, \alpha)), R_\gamma(U_2(n, \alpha))\}$ for $0 < \gamma < 1$, and (ii) $M_f(U) < \max \{M_f(U_1(n, \alpha)), M_f(U_2(n, \alpha))\}$ holds for any good escalating function $f(x, y)$.

Proof. In the proof of this result, denote by $\pi' = (\alpha + 1, 2^{(n-\alpha)}, 1^{(\alpha-1)})$ and $\pi'' = (\alpha, 3^{(2)}, 2^{(n-\alpha-3)}, 1^{(\alpha)})$. Since the deletion of any edge of the unique cycle of U forms a tree, we have $\alpha \geq \lceil \frac{n-1}{2} \rceil$. We suppose that the degree sequence of U is π , C_g is the unique cycle of U , and U contains p pendent vertices. By (2), $p \leq \alpha$.

Let U be a unicyclic graph of $\Gamma(\pi')$. If $g \geq 4$, then all the pendent vertices combining with at least two vertices of C_g will form an independent vertex set of size being at least $\alpha + 1$, a contradiction. Thus, the unique cycle of U is a triangle. Since U contains exactly $\alpha - 1$ pendent vertices, except for two adjacent 2-vertices in the triangle of U , each of the other 2-vertices is adjacent to at least one pendent vertex. By Lemma 3.4, we have $U \cong U_1(n, \alpha)$.

Let U be a unicyclic graph of $\Gamma(\pi'')$. Then, the class of pendent vertices of U form an independent vertex set of U , and hence every non-pendent vertex is adjacent to at least a pendent vertex. By Lemma 3.5, we have $U \cong U_2(n, \alpha)$.

Now, we can conclude that

$$\Gamma(\pi') = \{U_1(n, \alpha)\} \text{ and } \Gamma(\pi'') = \{U_2(n, \alpha)\}. \tag{7}$$

Since $U \notin \{U_1(n, \alpha), U_2(n, \alpha)\}$, we have $\pi \notin \{\pi', \pi''\}$.

If $p \leq \alpha - 1$, then $\pi \triangleleft \pi'$ by Lemma 3.1.

Otherwise, $p = \alpha$. Since $p = \alpha$, each non-pendent vertex is adjacent to at least a pendent vertex. By Lemma 3.2 (i), we have $\pi \triangleleft \pi''$.

By Theorem 2.2 and (7), the results hold. ■

Corollary 3.2 *Let U be a unicyclic graph with n vertices and independence number α ($\leq n - 3$) such that $U \not\cong U_1(n, \alpha)$. (i) If $\gamma > 1$ and $\alpha \geq 4$, then $\chi_\gamma(U) < \chi_\gamma(U_1(n, \alpha))$ and $Z_\gamma(U) < Z_\gamma(U_1(n, \alpha))$. (ii) If $\alpha \geq 4$, then $M_1(U) < M_1(U_1(n, \alpha))$. (iii) If $n \geq 9$ and $\alpha \geq 3$, then $M_2(U) < M_2(U_1(n, \alpha))$.*

Proof. By an elementary computation, it follows that

$$\begin{aligned} \chi_\gamma(U_1(n, \alpha)) &= (n - \alpha)(\alpha + 3)^\gamma + (2\alpha - n + 1)(\alpha + 2)^\gamma + 4^\gamma + (n - \alpha - 2)3^\gamma, \\ \chi_\gamma(U_2(n, \alpha)) &= 2(\alpha + 3)^\gamma + (n - \alpha - 3)(\alpha + 2)^\gamma + (2\alpha - n + 1)(\alpha + 1)^\gamma + 6^\gamma \end{aligned}$$

$$+ 2 \times 4^\gamma + (n - \alpha - 3)3^\gamma.$$

When $\gamma > 1$ and $\alpha \geq 4$, we have

$$\begin{aligned} \chi_\gamma(U_1(n, \alpha)) - \chi_\gamma(U_2(n, \alpha)) &= (\alpha + 3)^\gamma + (n - \alpha - 3) \left((\alpha + 3)^\gamma - (\alpha + 2)^\gamma \right) \\ &\quad + (2\alpha - n + 1) \times \left((\alpha + 2)^\gamma - (\alpha + 1)^\gamma \right) - 6^\gamma - 4^\gamma + 3^\gamma \\ &> 7^\gamma - 6^\gamma - 4^\gamma + 3^\gamma > 0 \end{aligned}$$

by Corollary 2.1. With the similar reason, we have $Z_\gamma(U_1(n, \alpha)) > Z_\gamma(U_2(n, \alpha))$.

Thus, (i) follows from Theorems 2.2 and 3.2.

It is easy to check that

$$M_1(U_1(n, \alpha)) - M_1(U_2(n, \alpha)) = 2(\alpha - 3) > 0$$

when $\alpha \geq 4$, and hence (ii) also follows from Theorems 2.2 and 3.2.

Now, we turn to prove (iii). Since

$$\begin{aligned} M_2(U_1(n, \alpha)) &= 2(\alpha + 1)(n - \alpha) + 4 + 2(n - \alpha - 2) + (\alpha + 1)(2\alpha + 1 - n) \\ &= n\alpha + 3n - \alpha + 1, \end{aligned}$$

$$\begin{aligned} \text{and } M_2(U_2(n, \alpha)) &= 2 \times 3\alpha + 15 + 2\alpha(n - \alpha - 3) + 2(n - \alpha - 3) + \alpha(2\alpha + 1 - n) \\ &= n\alpha + 2n - \alpha + 9. \end{aligned}$$

For $n \geq 9$, we have

$$M_2(U_1(n, \alpha)) - M_2(U_2(n, \alpha)) = n - 8 > 0,$$

and hence (iii) follows from Theorems 2.2 and 3.2. ■

Theorem 3.3 *Let B be a bicyclic graph with n vertices and independence number α , where $4 \leq \alpha \leq n - 4$.*

(i) *If $B \notin \{Z_1(n, \alpha), Z_2(n, \alpha), Z_3(n, \alpha), Z_4(n, \alpha)\}$, then*

$$R_\gamma(B) < \max \left\{ R_\gamma(Z_2(n, \alpha)), R_\gamma(Z_3(n, \alpha)), R_\gamma(Z_4(n, \alpha)) \right\}$$

holds for $\gamma < 0$ or $\gamma > 1$, and

$$R_\gamma(B) > \min \left\{ R_\gamma(Z_2(n, \alpha)), R_\gamma(Z_3(n, \alpha)), R_\gamma(Z_4(n, \alpha)) \right\}$$

holds for $0 < \gamma < 1$.

(ii) *If $B \notin \{Z_2(n, \alpha), Z_3(n, \alpha), Z_4(n, \alpha)\}$ and $f(x, y)$ is a good escalating function, then*

$$M_f(B) < \max \left\{ M_f(Z_2(n, \alpha)), M_f(Z_3(n, \alpha)), M_f(Z_4(n, \alpha)) \right\}.$$

Proof. Suppose C_s and C_t are two cycles of B , the degree sequence of B is $\pi = (d_1, d_2, \dots, d_n)$ and B contains p pendent vertices. By (2), $p \leq \alpha$. In the proof of this result, denote by $\pi' = (\alpha, 4, 3^{(2)}, 2^{(n-\alpha-4)}, 1^{(\alpha)})$, $\pi'' = (\alpha + 1, 3^{(2)}, 2^{(n-\alpha-2)}, 1^{(\alpha-1)})$ and $\pi''' = (\alpha + 2, 2^{(n-\alpha+1)}, 1^{(\alpha-2)})$.

Firstly, we suppose that $\pi = \pi'$. Since $p = \alpha$, every non-pendent vertex is adjacent to at least one pendent vertex. By Lemma 3.5, we have $B \cong Z_4(n, \alpha)$.

Secondly, we suppose that $\pi = \pi'''$. Since $d_2 = 2$, we have $|V(C_s) \cap V(C_t)| = 1$. Then, there is an independent set of size at least $\alpha - 2 + \lfloor \frac{\alpha}{2} \rfloor + \lfloor \frac{\alpha}{2} \rfloor$, and hence $s = t = 3$. Now, it is easy to see that there are exactly four 2-vertices being not adjacent to any pendent vertex in B . By Lemma 3.4, $B \cong Z_3(n, \alpha)$.

Thirdly, we suppose that $\pi = \pi''$. Since $p = \alpha - 1$, all the non-pendent vertices being not adjacent to any pendent vertex must induce a complete graph K_q . Recall that $\mathcal{R}(B)$ is also a bicyclic graph. Thus, $q \in \{0, 1, 2, 3\}$. We assume that $q \in \{0, 1\}$. Since $d_4 = 2$, we have $|V(C_s) \cup V(C_t)| = 4$ and there is exactly one non-pendent vertex being not adjacent to any pendent vertex, that is, $q = 1$. In this case, $\mathcal{R}(B) \cong K_4 - e$, and either $d_2 \geq 4$ or $d_4 \geq 3$ (since there is exactly one non-pendent vertex of B being not adjacent to any pendent vertex), a contradiction. Thus, $q \in \{2, 3\}$, that is, all the non-pendent vertices being not adjacent to any pendent vertex induce either K_2 or K_3 . By Lemma 3.6, $B \in \{Z_1(n, \alpha), Z_2(n, \alpha)\}$.

By an elementary computation, it follows that

$$M_f(Z_2(n, \alpha)) - M_f(Z_1(n, \alpha)) = f(3, 2) + f(2, 1) - f(2, 2) - f(3, 1) > 0$$

when $f(x, y)$ is a good escalating function. Combining this with the above arguments, we may suppose that $\pi \notin \{\pi', \pi'', \pi'''\}$. By Theorem 2.2, it suffices to show

$$\pi \triangleleft \pi' \text{ or } \pi \triangleleft \pi'' \text{ or } \pi \triangleleft \pi''' \tag{8}$$

If $p \leq \alpha - 2$, then $\pi \triangleleft \pi'''$ by Lemma 3.1 and hence (8) holds.

If $p = \alpha$, then every non-pendent vertex is adjacent to at least one pendent vertex. Now, Lemma 3.2 (ii) implies that $\pi \triangleleft \pi'$ and hence (8) holds.

If $p = \alpha - 1$, then all non-pendent vertices of B being not adjacent to any pendent vertex induce a complete graph K_q . Since $\mathcal{R}(B)$ is also a bicyclic graph, $q \in \{0, 1, 2, 3\}$. When $q \in \{0, 1\}$ or $|V(C_s) \cup V(C_t)| \geq 6$, then $d_3 \geq 3$. When $|V(C_s) \cup V(C_t)| = 5$ and $q \in \{2, 3\}$, we also have $d_3 \geq 3$. Otherwise, $|V(C_s) \cup V(C_t)| = 4$ and $q \in \{2, 3\}$. In this case, $\mathcal{R}(B) \cong K_4 - e$ and hence $d_3 \geq 3$. Now, Lemma 3.3 implies that $\pi \triangleleft \pi''$ and hence (8) holds. ■

Corollary 3.3 *Let B be a bicyclic graph with n vertices and independence number α such that $B \not\cong Z_3(n, \alpha)$. If $\gamma > 1$ and $5 \leq \alpha \leq n - 4$, then $\chi_\gamma(B) < \chi_\gamma(Z_3(n, \alpha))$ and $Z_\gamma(B) < Z_\gamma(Z_3(n, \alpha))$.*

Proof. By an elementary computation, it follows that

$$\begin{aligned} \chi_\gamma(Z_2(n, \alpha)) &= 2(\alpha + 4)^\gamma + (\alpha + 3)^\gamma(n - \alpha - 2) + (\alpha + 2)^\gamma(2\alpha - n + 1) \\ &\quad + 5^\gamma + 6^\gamma + 4^\gamma + 3^\gamma(n - \alpha - 3), \\ \chi_\gamma(Z_3(n, \alpha)) &= (\alpha + 4)^\gamma(n - \alpha + 1) + (\alpha + 3)^\gamma(2\alpha - n + 1) + 3^\gamma(n - \alpha - 3) + 4^\gamma \times 2, \\ \chi_\gamma(Z_4(n, \alpha)) &= (\alpha + 4)^\gamma + 2(\alpha + 3)^\gamma + (\alpha + 2)^\gamma(n - \alpha - 4) \\ &\quad + (\alpha + 1)^\gamma(2\alpha - n + 1) + 3^\gamma(n - \alpha - 4) + 7^\gamma \times 2 + 5^\gamma + 4^\gamma \times 2. \end{aligned}$$

For $\gamma > 1$, by Corollary 2.1 we have

$$\begin{aligned} &\chi_\gamma(Z_3(n, \alpha)) - \chi_\gamma(Z_2(n, \alpha)) \\ &= (\alpha + 4)^\gamma + (n - \alpha - 2) \left((\alpha + 4)^\gamma - (\alpha + 3)^\gamma \right) \\ &\quad + (2\alpha - n + 1) \left((\alpha + 3)^\gamma - (\alpha + 2)^\gamma \right) + 4^\gamma - 5^\gamma - 6^\gamma \\ &\geq (\alpha + 4)^\gamma + 4^\gamma - 5^\gamma - 6^\gamma \geq 7^\gamma + 4^\gamma - 5^\gamma - 6^\gamma > 0, \\ &\chi_\gamma(Z_2(n, \alpha)) - \chi_\gamma(Z_4(n, \alpha)) \\ &= (\alpha + 4)^\gamma + (n - \alpha - 4) \left((\alpha + 3)^\gamma - (\alpha + 2)^\gamma \right) \\ &\quad + (2\alpha - n + 1) \times \left((\alpha + 2)^\gamma - (\alpha + 1)^\gamma \right) + 3^\gamma + 6^\gamma - 7^\gamma \times 2 - 4^\gamma \\ &\geq (\alpha + 4)^\gamma + 3^\gamma + 6^\gamma - 7^\gamma \times 2 - 4^\gamma \\ &\geq 9^\gamma + 6^\gamma + 3^\gamma - 7^\gamma \times 2 - 4^\gamma > 0. \end{aligned}$$

Thus, $\chi_\gamma(Z_4(n, \alpha)) < \chi_\gamma(Z_2(n, \alpha)) < \chi_\gamma(Z_3(n, \alpha))$.

With the similar reason,

$$Z_\gamma(Z_4(n, \alpha)) < Z_\gamma(Z_2(n, \alpha)) < Z_\gamma(Z_3(n, \alpha)).$$

Now, the result follows from Theorems 2.3 and 3.3. ■

Corollary 3.4 *Let B be a bicyclic graph with n vertices and independence number α , where $4 \leq \alpha \leq n - 4$. If $n \geq 10$ and $B \not\cong Z_3(n, \alpha)$, then $M_2(B) < M_2(Z_3(n, \alpha))$.*

Proof. From the definition, it follows that

$$M_2(Z_4(n, \alpha)) = 4\alpha + 2 \times 3\alpha + 2\alpha(n - \alpha - 4) + \alpha(2\alpha - n + 1) + 2(n - \alpha - 4) + 34$$

$$\begin{aligned}
 &= \alpha n + 2n + \alpha + 26, \\
 M_2(Z_3(n, \alpha)) &= 2(\alpha + 2)(n - \alpha + 1) + (\alpha + 2)(2\alpha - n + 1) + 8 + 2(n - \alpha - 3) \\
 &= \alpha n + \alpha + 4n + 8, \\
 M_2(Z_2(n, \alpha)) &= \alpha n + 3n + \alpha + 15.
 \end{aligned}$$

Thus, $M_2(Z_3(n, \alpha)) - M_2(Z_2(n, \alpha)) = n - 7 > 0$ and $M_2(Z_3(n, \alpha)) - M_2(Z_4(n, \alpha)) = 2n - 18 > 0$.

Now, the result follows from Theorems 2.3 and 3.3. ■

4 Extremal results with given matching number

In this section, we will consider the extremal problem in the class of c -cyclic graph with n vertices and matching number β . To this aim, we rewrite $S_1(0; \beta - 1, n + 1 - 2\beta)$ as $T(n; \beta)$, $S_1(1; \beta - 2, n + 1 - 2\beta)$ as $U_1(n; \beta)$, $S_2(1; \beta - 3, n + 1 - 2\beta)$ as $U_2(n; \beta)$, $B_1(\beta - 2, n + 1 - 2\beta)$ as $Z_1(n; \beta)$, $B_2(\beta - 2, n + 1 - 2\beta)$ as $Z_2(n; \beta)$, $S_1(2; \beta - 3, n + 1 - 2\beta)$ as $Z_3(n; \beta)$, and rewrite $S_2(2; \beta - 4, n + 1 - 2\beta)$ as $Z_4(n; \beta)$.

Theorem 4.1 *Let T be a tree with $n (\geq 3)$ vertices and matching number β . If $T \not\cong T(n; \beta)$, then (i) $R_\gamma(T) < R_\gamma(T(n; \beta))$ holds for either $\gamma < 0$ or $\gamma > 1$, and $R_\gamma(T) > R_\gamma(T(n; \beta))$ holds for $0 < \gamma < 1$, and (ii) $M_f(T) < M_f(T(n; \beta))$ for any good escalating function $f(x, y)$.*

Proof. Suppose the degree sequence of T is π and $\pi' = (n - \beta, 2^{(\beta-1)}, 1^{(n-\beta)})$. Note that T contains at least β vertices of degree being at least two and $\beta \leq \lfloor \frac{n}{2} \rfloor$. Thus, $p(T) \leq n - \beta$ and hence $\pi \leq \pi'$ by Lemma 3.1 and (3). If $\pi = \pi'$, then T contains exactly β vertices with degree being at least two. Since the matching number of T is β , each non-pendent vertex is adjacent to at least one pendent vertex. By Lemma 3.4, we have $T \cong T(n; \beta)$, a contradiction. Thus, $\pi \triangleleft \pi'$ and hence the results follow from Theorem 2.2 and $\Gamma(\pi') = \{T(n; \beta)\}$. ■

Corollary 4.1 *Let T be a tree with $n (\geq 3)$ vertices and matching number β . If $T \not\cong T(n; \beta)$, then (i) $\chi_\gamma(T) < \chi_\gamma(T(n; \beta))$ and $Z_\gamma(T) < Z_\gamma(T(n; \beta))$ holds for $\gamma \geq 1$, (ii) $M_1(T) < M_1(T(n; \beta))$ and $M_2(T) < M_2(T(n; \beta))$, and (iii) $[12] ID(T) < ID(T(n; \beta))$.*

Proof. By Theorems 2.3 and 4.1, the results hold. ■

Theorem 4.2 *Let U be a unicyclic graph with n vertices and matching number β , where $3 \leq \beta \leq n-3$. If $U \notin \{U_1(n; \beta), U_2(n; \beta)\}$, then (i) $R_\gamma(U) < \max\{R_\gamma(U_1(n; \beta)), R_\gamma(U_2(n; \beta))\}$ for $\gamma < 0$ or $\gamma > 1$, and $R_\gamma(U) > \min\{R_\gamma(U_1(n; \beta)), R_\gamma(U_2(n; \beta))\}$ for $0 < \gamma < 1$, and (ii) $M_f(U) < \max\{M_f(U_1(n; \beta)), M_f(U_2(n; \beta))\}$ for any good escalating function.*

Proof. In the proof of this result, let $\pi' = (n - \beta, 3^{(2)}, 2^{(\beta-3)}, 1^{(n-\beta)})$ and $\pi'' = (n - \beta + 1, 2^{(\beta)}, 1^{(n-\beta-1)})$. Suppose that the degree sequence of U is π , C_g is the unique cycle of U , and U contains p pendent vertices. By (3), $p(U) \leq n - \beta$.

Firstly, we suppose that $U \in \Gamma(\pi')$. Then, every non-pendent vertex is adjacent to at least one pendent vertex (since U contains exactly $n - \beta$ pendent vertices and β non-pendent vertices). By Lemma 3.5, we have $U \cong U_2(n; \beta)$, a contradiction.

Secondly, we suppose that $U \in \Gamma(\pi'')$. By the definition of π'' , every vertex of $V(C_g) \setminus \{v_1\}$ cannot be adjacent to any pendent vertex. Note that there are $\beta + 1$ non-pendent vertices in U and every edge in a matching has at least one non-pendent vertex as its end vertex. If $g \geq 4$, then the matching number of U is at most $\lfloor \frac{g-1}{2} \rfloor + \beta + 1 - (g-1) \leq \beta - 1$, a contradiction. Thus, $g = 3$ and hence there are exactly two 2-vertices in C_g being not adjacent to any pendent vertex. By Lemma 3.4, we have $U \cong U_1(n; \beta)$, a contradiction.

From the above arguments, it follows that

$$\Gamma(\pi') = \{U_2(n; \beta)\} \text{ and } \Gamma(\pi'') = \{U_1(n; \beta)\}. \tag{9}$$

Now, we suppose that $\pi \notin \{\pi', \pi''\}$. If $p \leq n - \beta - 1$, then $\pi \triangleleft \pi''$ by Lemma 3.1. If $p = n - \beta$, then since every edge in a matching has at least one non-pendent vertex as its end vertex and the matching number of U is β , we can conclude that each non-pendent vertex is adjacent to at least one pendent vertex. By Lemma 3.2 (i), it follows that $\pi \triangleleft \pi'$.

By Theorem 2.2 and (9), the results hold. ■

Corollary 4.2 *Let U be a unicyclic graph with n vertices and matching number $\beta (\geq 3)$ such that $U \not\cong U_1(n; \beta)$. (i) If $\gamma > 1$ and $\beta \leq n - 4$, then $\chi_\gamma(U) < \chi_\gamma(U_1(n; \beta))$, $Z_\gamma(U) < Z_\gamma(U_1(n; \beta))$ and $M_1(U) < M_1(U_1(n; \beta))$. (ii) If $n \geq 9$ and $\beta \leq n - 3$, then $M_2(U) < M_2(U_1(n; \beta))$.*

Proof. By an elementary computation, we have

$$\chi_\gamma(U_1(n; \beta)) = \beta(n - \beta + 3)^\gamma + (n - 2\beta + 1)(n - \beta + 2)^\gamma + 4^\gamma + (\beta - 2)3^\gamma,$$

and

$$\begin{aligned} \chi_\gamma(U_2(n; \beta)) &= 2(n - \beta + 3)^\gamma + (\beta - 3) ((n - \beta + 2)^\gamma + 3^\gamma) + (n - 2\beta + 1)(n - \beta + 1)^\gamma \\ &\quad + 6^\gamma + 2 \times 4^\gamma. \end{aligned}$$

We first prove (i). Since $\gamma > 1$ and $3 \leq \beta \leq n - 4$,

$$\begin{aligned} \chi_\gamma(U_1(n; \beta)) - \chi_\gamma(U_2(n; \beta)) &= (n - \beta + 3)^\gamma + (\beta - 3) ((n - \beta + 3)^\gamma - (n - \beta + 2)^\gamma) \\ &\quad + (n - 2\beta + 1) ((n - \beta + 2)^\gamma - (n - \beta + 1)^\gamma) - 6^\gamma - 4^\gamma \\ &\quad + 3^\gamma > 7^\gamma - 6^\gamma - 4^\gamma + 3^\gamma > 0 \end{aligned}$$

by Corollary 2.1. With the similar reason, $Z_\gamma(U_2(n; \beta)) < Z_\gamma(U_1(n; \beta))$. It is easy to see that

$$M_1(U_1(n; \beta)) - M_1(U_2(n; \beta)) = 2(n - \beta - 3) > 0.$$

Thus, (i) follows from Theorems 2.3 and 4.2.

Now, we turn to prove (ii). By Theorems 2.3 and 4.2, it suffices to show that $M_2(U_1(n; \beta)) > M_2(U_2(n; \beta))$. By an elementary computation, we have

$$\begin{aligned} M_2(U_1(n; \beta)) &= 2\beta(n - \beta + 1) + 4 + 2(\beta - 2) + (n - \beta + 1)(n - 2\beta + 1) \\ &= n^2 - n\beta + \beta + 2n + 1, \end{aligned}$$

$$\begin{aligned} M_2(U_2(n; \beta)) &= 2 \times 3(n - \beta) + 15 + 2(n - \beta)(\beta - 3) + 2(\beta - 3) + (n - \beta)(n - 2\beta + 1) \\ &= n^2 - n\beta + \beta + n + 9. \end{aligned}$$

Thus, $M_2(U_1(n; \beta)) - M_2(U_2(n; \beta)) = n - 8 > 0$. ■

Theorem 4.3 *Let B be a bicyclic graph with n vertices and matching number β , where $4 \leq \beta \leq n - 4$.*

(i) *If $B \notin \{Z_1(n; \beta), Z_2(n; \beta), Z_3(n; \beta), Z_4(n; \beta)\}$, then*

$$R_\gamma(B) < \max \left\{ R_\gamma(Z_2(n; \beta)), R_\gamma(Z_3(n; \beta)), R_\gamma(Z_4(n; \beta)) \right\}$$

holds for $\gamma < 0$ or $\gamma > 1$, and

$$R_\gamma(B) > \min \left\{ R_\gamma(Z_2(n; \beta)), R_\gamma(Z_3(n; \beta)), R_\gamma(Z_4(n; \beta)) \right\}$$

holds for $0 < \gamma < 1$.

(ii) *If $B \notin \{Z_2(n; \beta), Z_3(n; \beta), Z_4(n; \beta)\}$ and $f(x, y)$ is a good escalating function, then*

$$M_f(B) < \max \left\{ M_f(Z_2(n; \beta)), M_f(Z_3(n; \beta)), M_f(Z_4(n; \beta)) \right\}.$$

Proof. Suppose C_s and C_t are two cycles of B , the degree sequence of B is $\pi = (d_1, d_2, \dots, d_n)$ and B contains p pendent vertices. By (3), $p \leq n - \beta$. In the proof of this result, denote by $\pi' = (n - \beta, 4, 3^{(2)}, 2^{(\beta-4)}, 1^{(n-\beta)})$, $\pi'' = (n - \beta + 1, 3^{(2)}, 2^{(\beta-2)}, 1^{(n-\beta-1)})$ and $\pi''' = (n - \beta + 2, 2^{(\beta+1)}, 1^{(n-\beta-2)})$.

Firstly, we suppose that $\pi = \pi'$. Since B contains exactly β non-pendent vertices and the matching number of B is equal to β , every non-pendent vertex is adjacent to at least one pendent vertex. By Lemma 3.5, we have $B \cong Z_4(n; \beta)$.

Secondly, we suppose that $\pi = \pi'''$. Since $d_2 = 2$, we have $|V(C_s) \cap V(C_t)| = 1$. Note that there are at most $\lfloor \frac{s-1}{2} \rfloor + \lfloor \frac{t-1}{2} \rfloor$ independent edges induced by the vertex set $(V(C_s) \cup V(C_t)) \setminus \{v_1\}$. Thus, the matching number of B is at most

$$\beta + \left\lfloor \frac{s-1}{2} \right\rfloor + \left\lfloor \frac{t-1}{2} \right\rfloor + 2 - (s-1 + t-1) \leq \beta + 2 - \left\lceil \frac{s-1}{2} \right\rceil - \left\lceil \frac{t-1}{2} \right\rceil \leq \beta,$$

and hence $s = t = 3$. Since the matching number of B is equal to β , B contains exactly four 2-vertices being not adjacent to any pendent vertex in B . By Lemma 3.4, $B \cong Z_3(n; \beta)$.

Thirdly, we suppose that $\pi = \pi''$. Since B contains $\beta+1$ non-pendent vertices and each edge of the maximum matching with β edges in B contains at least one non-pendent vertex as its end vertex, there is either at most one non-pendent vertex being not adjacent to any pendent vertex or there are exactly two adjacent non-pendent vertices being not adjacent to any pendent vertex. Now, we assume that there is at most one non-pendent vertex being not adjacent to any pendent vertex. Since $d_4 = 2$, we have $|V(C_s) \cup V(C_t)| = 4$ and there is exactly one non-pendent vertex being not adjacent to any pendent vertex. In this case, it follows that $\mathcal{R}(B) \cong K_4 - e$, and hence either $d_2 \geq 4$ or $d_4 \geq 3$ (since there is exactly one non-pendent vertex of B being not adjacent to any pendent vertex), a contradiction. Thus, there are exactly two adjacent non-pendent vertices being not adjacent to any pendent vertex. By Lemma 3.6, $B \in \{Z_1(n; \beta), Z_2(n; \beta)\}$.

By an elementary computation, it follows that

$$M_f(Z_2(n; \beta)) - M_f(Z_1(n; \beta)) = f(3, 2) + f(2, 1) - f(2, 2) - f(3, 1) > 0$$

when $f(x, y)$ is a good escalating function. Combining this with the above arguments, we may suppose that $\pi \notin \{\pi', \pi'', \pi'''\}$. By Theorem 2.2, it suffices to show

$$\pi \triangleleft \pi' \text{ or } \pi \triangleleft \pi'' \text{ or } \pi \triangleleft \pi''' \tag{10}$$

If $p \leq n - \beta - 2$, then $\pi \triangleleft \pi'''$ by Lemma 3.1 and hence (10) holds.

If $p = n - \beta$, then every non-pendent vertex is adjacent to at least one pendent vertex. Now, Lemma 3.2 (ii) implies that $\pi \triangleleft \pi'$ and hence (10) holds.

If $p = n - \beta - 1$, then B contains exactly $\beta + 1$ non-pendent vertices. In this case, either at most one non-pendent vertex being not adjacent to any pendent vertex or there exist two adjacent non-pendent vertices being not adjacent to any pendent vertex. When $|V(C_s) \cup V(C_t)| \geq 5$, then $d_3 \geq 3$. Otherwise, $|V(C_s) \cup V(C_t)| = 4$ and hence $\mathcal{R}(B) \cong K_4 - e$. Recall that either at most one non-pendent vertex is not adjacent to any pendent vertex or there exist two adjacent non-pendent vertices being not adjacent to any pendent vertex. Thus, $d_3 \geq 3$. Now, Lemma 3.3 implies that $\pi \triangleleft \pi''$ and hence (10) holds. ■

Corollary 4.3 *Let B be a bicyclic graph with n vertices and matching number β such that $B \not\cong Z_3(n; \beta)$. If $\gamma > 1$ and $4 \leq \beta \leq n - 4$, then $\chi_\gamma(B) < \chi_\gamma(Z_3(n; \beta))$ and $Z_\gamma(B) < Z_\gamma(Z_3(n; \beta))$.*

Proof. By an elementary computation, it follows that

$$\begin{aligned} \chi_\gamma(Z_2(n, \alpha)) &= 2(n - \beta + 4)^\gamma + (n - \beta + 3)^\gamma(\beta - 2) + (n - \beta + 2)^\gamma(n - 2\beta + 1) \\ &\quad + 5^\gamma + 6^\gamma + 4^\gamma + 3^\gamma(\beta - 3), \end{aligned}$$

$$\begin{aligned} \chi_\gamma(Z_3(n; \beta)) &= (n - \beta + 4)^\gamma(\beta + 1) + (n - \beta + 3)^\gamma(n - 2\beta + 1) + 3^\gamma(\beta - 3) \\ &\quad + 4^\gamma \times 2, \end{aligned}$$

$$\begin{aligned} \text{and } \chi_\gamma(Z_4(n; \beta)) &= (n - \beta + 4)^\gamma + 2(n - \beta + 3)^\gamma + (n - \beta + 2)^\gamma(\beta - 4) \\ &\quad + (n - \beta + 1)^\gamma(n - 2\beta + 1) + 3^\gamma(\beta - 4) + 7^\gamma \times 2 + 5^\gamma + 4^\gamma \times 2. \end{aligned}$$

Since $\gamma > 1$ and $4 \leq \beta \leq n - 4$, by Corollary 2.1 we have

$$\begin{aligned} \chi_\gamma(Z_3(n; \beta)) - \chi_\gamma(Z_2(n; \beta)) &= (n - \beta + 4)^\gamma + (\beta - 2) \left((n - \beta + 4)^\gamma - (n - \beta + 3)^\gamma \right) \\ &\quad + (n - 2\beta + 1) \times \left((n - \beta + 3)^\gamma - (n - \beta + 2)^\gamma \right) + 4^\gamma \\ &\quad - 5^\gamma - 6^\gamma \end{aligned}$$

$$\geq (n - \beta + 4)^\gamma + 4^\gamma - 5^\gamma - 6^\gamma \geq 7^\gamma + 4^\gamma - 5^\gamma - 6^\gamma > 0,$$

$$\begin{aligned} \chi_\gamma(Z_3(n; \beta)) - \chi_\gamma(Z_4(n; \beta)) &= (n - \beta + 4)^\gamma \times 2 + (\beta - 4) \left((n - \beta + 4)^\gamma - (n - \beta + 2)^\gamma \right) \\ &\quad + (n - 2\beta + 1) \left((n - \beta + 3)^\gamma - (n - \beta + 1)^\gamma \right) \\ &\quad + 2 \left((n - \beta + 4)^\gamma - (n - \beta + 3)^\gamma \right) + 3^\gamma - 7^\gamma \times 2 - 5^\gamma \\ &\geq 2(n - \beta + 4)^\gamma + 3^\gamma - 7^\gamma \times 2 - 5^\gamma \geq 8^\gamma \times 2 + 3^\gamma - 7^\gamma \times 2 \\ &\quad - 5^\gamma > 0. \end{aligned}$$

Thus, $\max \left\{ \chi_\gamma(Z_2(n; \beta)), \chi_\gamma(Z_4(n; \beta)) \right\} < \chi_\gamma(Z_3(n; \beta))$.

With the similar reason,

$$\max \left\{ Z_\gamma(Z_2(n; \beta)), Z_\gamma(Z_4(n; \beta)) \right\} < Z_\gamma(Z_3(n; \beta)).$$

Now, the result follows from Theorems 2.3 and 4.3. ■

Corollary 4.4 *Let B be a bicyclic graph with n vertices and matching number β , where $4 \leq \beta \leq n - 4$. If $n \geq 10$ and $B \not\cong Z_3(n; \beta)$, then $M_2(B) < M_2(Z_3(n; \beta))$.*

Proof. By an elementary computation, it follows that

$$\begin{aligned} M_2(Z_2(n; \beta)) &= 6(n - \beta + 1) + 2(n - \beta + 1)(\beta - 2) + (n - \beta + 1)(n - 2\beta + 1) + 18 \\ &\quad + 2(\beta - 3) \\ &= n^2 - \beta n - \beta + 4n + 15, \\ M_2(Z_3(n; \beta)) &= 2(n - \beta + 2)(\beta + 1) + (n - \beta + 2)(n - 2\beta + 1) + 8 + 2(\beta - 3) \\ &= n^2 - \beta n - \beta + 5n + 8, \\ M_2(Z_4(n; \beta)) &= 4(n - \beta) + 6(n - \beta) + 2(n - \beta)(\beta - 4) + (n - \beta)(n - 2\beta + 1) \\ &\quad + 2(\beta - 4) + 34 \\ &= n^2 - \beta n - \beta + 3n + 26. \end{aligned}$$

Since $M_2(Z_3(n; \beta)) - M_2(Z_2(n; \beta)) = n - 7 > 0$ and $M_2(Z_3(n; \beta)) - M_2(Z_4(n; \beta)) = 2n - 18 > 0$, the result follows from Theorems 2.3 and 4.3. ■

Acknowledgment: The authors are grateful to the anonymous referee for helpful suggestions and valuable comments, which led to an improvement of the original manuscript. The second author is partially supported by NNSF of China (No. 11571123), the Training Program for Outstanding Young Teachers in University of Guangdong Province (No. YQ2015027), Guangdong Engineering Research Center for Data Science (No. 2017A-KF02), and The third author was supported by the Sungkyun research fund, Sungkyunkwan University, 2017, and National Research Foundation of the Korean government with grant No. 2017R1D1A1B03028642.

References

- [1] K. C. Das, K. Xu, I. Gutman, On Zagreb and Harary indices, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 301–314.
- [2] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.
- [3] G. H. Hardy, J. E. Littlewood, G. Pólya, *Inequalities*, Cambridge Univ. Press, Cambridge, 1952.
- [4] X. Li, J. Zheng, A unified approach to the extremal trees for different indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 195–208.
- [5] M. Liu, B. Liu, Some properties of the first general Zagreb index, *Australas. J. Comb.* **47** (2010) 285–294.
- [6] M. Liu, B. Liu, K.C. Das, Recent results on the majorization theory of graph spectrum and topological index theory—a survey, *El. J. Lin. Algebra* **30** (2015) 402–421.
- [7] M. Liu, K. Xu, X.-D. Zhang, Extremal graphs for vertex-degree-based invariants with given degree sequences, *submitted*.
- [8] A. W. Marshall, I. Olkin, *Inequalities: Theory of Majorization and its Applications*, Acad. Press, New York, 1979.
- [9] A. Miličević, S. Nikolić, N. Trinajstić, On reformulated Zagreb indices, *Mol. Diversity* **8** (2004) 393–399.
- [10] H. Wang, Functions on adjacent vertex degrees of trees with given degree sequence, *Central Eur. J. Math.* **12** (2014) 1656–1663.
- [11] I. Tomescu, M. K. Jamil, Maximum general sum-connectivity index for trees with given independence number, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 715–722.
- [12] K. Xu, K. C. Das, Some extremal graphs with respect to inverse degree, *Discr. Appl. Math.* **203** (2016) 171–183.
- [13] X. D. Zhang, Extremal graph theory for degree sequences, *arXiv* 1510.01903v1 [math.co], 2015.
- [14] B. Zhou, N. Trinajstić, On general sum-connectivity index, *J. Math. Chem.* **47** (2010) 210–218.