MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **82** (2019) 699-714

ISSN 0340 - 6253

Unified Extremal Results for Vertex–Degree–Based Graph Invariants with Given Diameter

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(Received March 5, 2019)

Abstract

In this paper, we determine all unified extremal graphs for maximum (resp., minimum) first general Zagreb index $R_\alpha^0(G)$ for $\alpha < 0$ or $\alpha > 1$ (resp., $0 < \alpha < 1$), maximum (resp., minimum) general first multiplicative Zagreb index $\prod^{\alpha}(G)$ for $\alpha < 0$ (resp., $\alpha > 0$), maximum second multiplicative Zagreb index $\prod_2(G)$, and minimum first Zagreb coindex $\overline{M_1(G)}$ among the class of trees, unicyclic graphs and bicyclic graphs with given diameter, respectively.

1 Introduction

In this paper, we only consider simple connected undirected graphs. Throughout the paper, α always denotes a real number and c is a nonnegative integer. Let $G = (V, E)$ be a connected graph with n vertices and m edges. If $m = n + c - 1$, then G is called a *c-cyclic graph*. A c-cyclic graph with $c = 0, 1, 2$ is called a *tree*, *unicyclic graph* and *bicyclic graph*, respectively. As usual, $d_G(u)$ or $d(u)$ for short, denotes the degree of u in G. A *k-vertex* is a vertex with degree k. A 1-vertex is called a *pendant vertex* of G, while a k-vertex with $k \geq 2$ is called a *non-pendant vertex*. The number of pendant vertices of G will be referred as $p(G)$ throughout this paper.

Suppose that $V(G) = \{v_1, v_2, \ldots, v_n\}$ with $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$. Let $d(v_i) = d_i$ for $i = 1, 2, \ldots, n$. The non-increasing sequence $\pi(G) = (d_1, d_2, \ldots, d_n)$ is called the *degree sequence* of G. Denote by $\Gamma(\pi)$ the set of all connected graphs with degree sequence π. If G is a c-cyclic graph with degree sequence π, then

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

The *distance* between u and v, denoted by $\mathrm{dist}(u, v)$, is the number of edges in a shortest path from u to v. Then, the *diameter* $d(G)$ of graph G is the maximum distance over all pairs of vertices of G.

In 1972, Gutman and Trinajstić [4] introduced the first Zagreb index, where the *first Zagreb index* $M_1(G)$ of a graph G equals to the sum of the squares of the degrees of all vertices of G. This topological index has been widely studied [3]. The *first Zagreb coindex* $\overline{M_1(G)}$ of a graph G defined by Došlić [2] is

$$\overline{M_1(G)} = \sum_{uv \notin E(G)} \big(d(u) + d(v)\big).$$

As a generalization of the first Zagreb index, the *first general Zagreb index* $R_\alpha(G)$ was introduced by Li and Zheng [7] which is defined as

$$R_\alpha^0(G) = \sum_{u \in V(G)} \big(d(u)\big)^\alpha.$$

In particular, $R_{-1}^0(G)$ is called the *inverse degree* of G and denoted by $ID(G)$ (see [18]); and $R_2^0(G)$ is just the first Zagreb index.

In 2010, Todeschini and Consonni [16] put forward the notations of the *first multiplicative Zagreb index* $\prod^{1}(G)$ and the *second multiplicative Zagreb index* $\prod_{2}(G)$ of graph G, where

$$\prod^{1}(G) = \prod_{u \in V(G)} d^2(u), \text{ and } \prod_{2}(G) = \prod_{u \in V(G)} \big(d(u)\big)^{d(u)}.$$

Very recently, the *general first multiplicative Zagreb index* $\prod^{\alpha}(G)$ was defined in [20] as

$$\prod^{\alpha}(G) = \prod_{u \in V(G)} \big(d(u)\big)^\alpha.$$

It is not hard to see that $\prod^{\alpha}(G)$ is a generalization of the first multiplicative Zagreb index.

To unify the vertex-degree-based topological indices, the *vertex-degree-function index* $H_f(G)$ of a graph G was constructed in [20], where

$$H_f(G) = \sum_{v \in V(G)} f\big(d(v)\big)$$

for a function $f(x)$ defined on positive real numbers.

Definition 1.1 *For a graph family $\mathcal{G}$, a graph $G \in \mathcal{G}$ is called a* good extremal graph *of $\mathcal{G}$ if*

(i) $R^0_\alpha(G)$ is maximum for $\alpha < 0$ or $\alpha > 1$, and $R^0_\alpha(G)$ is minimum for $0 < \alpha < 1$.

(ii) $\prod^{\alpha}(G)$ is maximum for $\alpha < 0$, and $\prod^{\alpha}(G)$ is minimum for $\alpha > 0$.

(iii) $\prod_2(G)$ is maximum and $\overline{M_1(G)}$ is minimum.

Extremal ordering problem is an important topic on topological indices. As observed in some literatures ([10, 19] for instance), many topological indices share the same extremal graphs. Thus, it is rather interesting for us to determine unified extremal graphs for as many topological indices as possible in a given graph family [8, 19, 20]. As extremal ordering problem for some topological indices in the class of c-cyclic graphs with a given diameter always attract much attention [6, 9, 17, 21], we shall identify all good extremal graphs in the class of c-cyclic graphs with given diameter for $c \in \{0, 1, 2\}$. Theorems 2.1, 2.2 and 2.3 are main results in this paper.

2 The main results

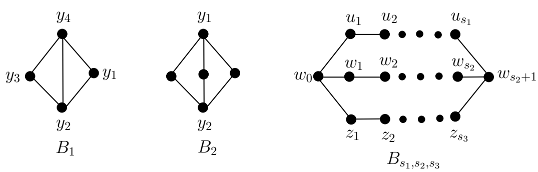

Figure 1. The bicyclic graphs B_1, B_2 and B_{s_1,s_2,s_3}

In this section, we shall introduce the main results of this paper, and we need to introduce more notations. As usual, the cycle and path with n vertices will be referred as C_n and P_n, respectively. Let G be a connected graph with $v \in V(G)$, and let P_k be a path on k vertices such that G and P_k are vertex-disjoint. Let G^* be a graph obtained from G and P_k by adding one edge between v and one end vertex of P_k. In this way, we say that G^* is obtained by *attaching* the path P_k to vertex v of G.

Hereafter, we suppose that d is the diameter of G. Let $x_0, x_d \in V(G)$ with $dist\big(x_0, x_d\big)$ $= d$ and $P_{d+1} = x_0 x_1 \ldots x_d$ denote a shortest path from x_0 to x_d. Define by $T_j(n, d)$ the tree obtained from P_{d+1} by attaching $n-d-1$ isolated vertices to x_j, where $1 \le j \le d-1$.

Theorem 2.1 *A tree T with n vertices and diameter d is a good extremal tree if and only if $T \in \Big\{T_1(n, d), T_2(n, d), \ldots, T_{\lfloor \frac{d}{2} \rfloor}(n, d)\Big\}$.*

If U is a unicyclic graph, then we let $C_g = z_1 z_2 \ldots z_g z_1$ be the unique cycle of U. For $1 \le j \le d-2$, let $U_{1,j}(n, d)$ be the unicyclic graph obtained from C_3 by attaching $n-d-2$ isolated vertices together with the path P_j with j vertices to z_1, and then attaching another path P_{d-j-1} with $d-j-1$ vertices to z_2. For $1 \le j \le d-3$, let $U_{2,j}(n, d)$ be the unicyclic graph obtained from C_4 by attaching $n-d-2$ isolated vertices together with the path P_j with j vertices to z_1, and then attaching another path P_{d-j-2} with $d-j-2$ vertices to z_3.

Theorem 2.2 *Let U be a unicyclic graph in the class of unicyclic graphs with n vertices and diameter d. If $4 \le d \le n-2$, then U is a good extremal unicyclic graph if and only if $U \in \big\{U_{1,1}(n, d), U_{1,2}(n, d), \ldots, U_{1,d-2}(n, d), U_{2,1}(n, d), U_{2,2}(n, d), \ldots, U_{2,d-3}(n, d)\big\}$.*

Hereafter, denote by B_1, B_2 and B_{s_1,s_2,s_3} the three bicyclic graphs as shown in Fig. 1. Let $B_{1,j}(n, d)$ be the bicyclic graph obtained from B_1 by attaching $n-d-2$ isolated vertices together with a path with j vertices to y_1 and then attaching another path with $d-j-2$ vertices to y_3, where $1 \le j \le d-3$. Let $B_{2,j}(n, d)$ be the bicyclic graph obtained from B_1 by attaching $n-d-2$ isolated vertices to y_2, a path with j vertices to y_1 and then attaching another path with $d-j-2$ vertices to y_3, where $1 \le j \le d-3$. Let $B_{3,j}(n, d)$ be the bicyclic graph obtained from B_1 by attaching $n-d-3$ isolated vertices together with a path with j vertices to y_2 and then attaching another path with $d-j-1$ vertices to y_4, where $1 \le j \le d-2$. Let $B_{4,j}(n, d)$ be the bicyclic graph obtained from B_2 by attaching $n-d-3$ isolated vertices together with a path with j vertices to y_1 and then attaching another path with $d-j-2$ vertices to y_2, where $1 \le j \le d-3$.

Theorem 2.3 *If $4 \leq d \leq n-3$ and B is a good extremal bicyclic graph in the class of bicyclic graphs with n vertices and diameter d, then either $B \in \{B_{1,i}(n,d), B_{2,j}(n,d)$, where $1 \leq i \leq d-3$ and $1 \leq j \leq \lfloor \frac{d}{2} \rfloor - 1\}$ or $B \in \{B_{3,k}(n,d), B_{4,i}(n,d)$, where $1 \leq i \leq d-3$ and $1 \leq k \leq d-2\}$.*

3 Some preliminaries

Let $\mathbf{s} = (s_1, s_2, ..., s_n)$ and $\mathbf{t} = (t_1, t_2, ..., t_n)$ be two non-increasing sequences of real numbers. We write $\mathbf{s} \trianglelefteq \mathbf{t}$ if and only if $\sum_{i=1}^{n} s_i = \sum_{i=1}^{n} t_i$, and $\sum_{i=1}^{j} s_i \leq \sum_{i=1}^{j} t_i$ for all $j = 1, 2, ..., n$. Furthermore, we write $\mathbf{s} \triangleleft \mathbf{t}$ if and only if $\mathbf{s} \trianglelefteq \mathbf{t}$ and $\mathbf{s} \neq \mathbf{t}$. The ordering $\mathbf{s} \trianglelefteq \mathbf{t}$ is always referred to as *majorization* [5, 12, 15].

A *strictly convex function* is a real valued function $g(x)$ defined on a convex set D such that

$$g\big(px + (1-p)y\big) < pg(x) + (1-p)g(y)$$

for all $0 < p < 1$ and all x, $y \in D$. Among all majorization theorems, the following one was discovered long time ago, and it is not restricted to graphical invariants.

Theorem 3.1 [15] *Let $\mathbf{s} = (s_1, s_2, ..., s_n)$ and $\mathbf{t} = (t_1, t_2, ..., t_n)$ be two non-increasing sequences of real numbers. If $\mathbf{s} \triangleleft \mathbf{t}$, then for any strictly convex function $g(x)$, we have $\sum_{i=1}^{n} g(s_i) < \sum_{i=1}^{n} g(t_i)$.*

Note that $-f(x)$ is a strictly convex function if and only if $f(x)$ is a strictly concave function. Thus, the following theorem easily follows from Theorem 3.1.

Theorem 3.2 [14, 20] *Let π and π' be two different non-increasing degree sequences with $\pi \triangleleft \pi'$, and G and G' be two graphs with $G \in \Gamma(\pi)$ and $G' \in \Gamma(\pi')$.*

(i) If $f(x)$ is a strictly convex function on $x \geq 1$, then $H_f(G) < H_f(G')$;

(ii) If $f(x)$ is a strictly concave function on $x \geq 1$, then $H_f(G) > H_f(G')$.

The following two results can be deduced from Theorems 3.1 and 3.2:

Theorem 3.3 [14, 20] *In a given graph family $\mathcal{G}$, if $H_f(G)$ is maximum for any strictly convex function on $x \geq 1$, then $R^0_\alpha(G)$ is maximum for $\alpha > 1$ or $\alpha < 0$, $\prod^{\alpha}(G)$ is maximum for $\alpha < 0$, $\prod_2(G)$ is maximum, and $\overline{M_1(G)}$ is minimum.*

Theorem 3.4 [14, 20] *In a given graph family $\mathcal{G}$, if $H_f(G)$ is minimum for any strictly concave function on $x \geq 1$, then $R^0_\alpha(G)$ is minimum for $0 < \alpha < 1$, and $\prod^{\alpha}(G)$ is minimum for $\alpha > 0$.*

4 The proof of Theorem 2.1

Let $\mathbb{C}(n, d, p; c)$ be the set of c-cyclic graphs with n vertices, p pendant vertices and diameter d. We will use the symbol $p^{(q)}$ to define q copies of the real number p. In what follows, denote by

$$\pi_1 = \left(n-d+1, 2^{(d-2)}, 1^{(n-d+1)}\right), \pi_2 = \left(n-d+1, 3, 2^{(d-2)}, 1^{(n-d)}\right),$$
$$\pi_3 = \left(n-d+1, 3^{(3)}, 2^{(d-4)}, 1^{(n-d)}\right), \text{and } \pi_4 = \left(n-d+1, 4, 2^{(d-1)}, 1^{(n-d-1)}\right).$$

Lemma 4.1 *If $T \in \mathbb{C}(n, d, p; 0)$, then $p \leq n-d+1$, where the equality holds if and only if T is obtained from P_{d+1} by attaching $n-d-1$ isolated vertices to some vertices of $\{x_1, x_2, \ldots, x_{d-1}\}$.*

Proof. If $T \in \mathbb{C}(n, d, p; 0)$, that is, T is a tree with n vertices, p pendant vertices and diameter d, then since there are at least $d-1$ non-pendant vertices on P_{d+1}, we have $p \leq n-d+1$. From this fact, it is straightly to verify this lemma. ■

Lemma 4.2 *Let $T \in \mathbb{C}(n, d, p; 0)$. If $\pi \neq \pi_1$ and $d \geq 2$, then $\pi \lhd \pi_1$.*

Proof. Let $\pi = \left(d_1, d_2, \ldots, d_{n-p}, 1^{(p)}\right)$, where $d_1 \geq d_2 \geq \cdots \geq d_{n-p} \geq 2$. Recall that $\pi_1 = \left(n-d+1, 2^{(d-2)}, 1^{(n-d+1)}\right)$. We assume that $\pi_1 = \left(d'_1, d'_2, \ldots, d'_{d-1}, 1^{(n-d+1)}\right)$, that is, $d'_1 = n-d+1$ and $d'_i = 2$ for $2 \leq i \leq d-1$.

Since T is a tree, by Lemma 4.1, we have

$$d_1 = 2(n-1) - p - d_2 - d_3 - \cdots - d_{n-p} \leq 2(n-1) - p - 2\left(n-p-1\right) = p \leq n-d+1.$$

If $d_1 = n-d+1$, then $d_2 = d_3 = \cdots = d_{n-p} = 2$, and hence $\pi = \pi_1$, a contradiction. Consequently, $d_1 < n-d+1$.

For $2 \leq j \leq d-1$, since $d_j \geq 2$ and $p \leq n-d+1$, by Lemma 4.1, we have

$$\begin{aligned}\sum_{i=1}^{j} d_i &= 2(n-1) - p - d_{j+1} - \cdots - d_{n-p} \\ &\leq 2(n-1) - p - 2\left(n-p-j\right) = p + 2j - 2 \leq n-d-1+2j = \sum_{i=1}^{j} d'_i.\end{aligned}$$

For $d \le j \le n$, since $d'_d = 1 \le d_d$, we have $\sum_{i=1}^{j} d_i \le 2(n-1)-(n-j) = n+j-2 = \sum_{i=1}^{j} d'_i$. Combining the above arguments, we have $\pi \lhd \pi_1$. ■

For simplification, let $\mathbb{T}(n,d)$ be the set of trees with n vertices, diameter d and degree sequence π_1, and $\mathbb{U}(n,d)$ be the set of unicyclic graphs with n vertices, diameter d and degree sequence π_2. Define $\mathbb{B}_1(n,d)$ $\big($resp., $\mathbb{B}_2(n,d)\big)$ as the set of bicyclic graphs with n vertices, diameter d and degree sequence π_3 $\big($resp., $\pi_4\big)$.

Lemma 4.3 *If $d \ge 2$, then $\mathbb{T}(n,d) = \Big\{T_1(n,d), T_2(n,d), \dots, T_{\lfloor \frac{d}{2} \rfloor}(n,d)\Big\}$.*

Proof. From the definition of $T_i(n,d)$, where $1 \le i \le d-1$,

$$\Big\{T_1(n,d), T_2(n,d), \dots, T_{\lfloor \frac{d}{2} \rfloor}(n,d)\Big\} \subseteq \mathbb{T}(n,d),$$

and so it suffices to show that $\mathbb{T}(n,d) \subseteq \Big\{T_1(n,d), T_2(n,d), \dots, T_{\lfloor \frac{d}{2} \rfloor}(n,d)\Big\}$.

Suppose that $T \in \mathbb{T}(n,d)$. By Lemma 4.1, T is obtained from P_{d+1} by attaching $n-d-1$ isolated vertices to some vertices of $\big\{x_1, x_2, \dots, x_d\big\}$. Since $d_1 = n-d+1$ by the definition of π_1, then all these $n-d-1$ isolated vertices are adjacent to the same vertex x_i, where $1 \le i \le d-1$. Since $T_i(n,d) = T_{d-i}(n,d)$, we can conclude that $T = T_j(n,d)$ for some $j \in \big\{1, 2, \dots, \lfloor \frac{d}{2} \rfloor\big\}$. ■

Now it is ready to present the following proof of Theorem 2.1.

Proof of Theorem 2.1. In view of Theorems 3.3 and 3.4, it suffices to show that T has the maximum (resp., minimum) $H_f(T)$ if $f(x)$ is a strictly convex (resp., concave) function on $x \ge 1$. We suppose that the degree sequence of T is π. By Lemma 4.2, $\pi \lhd \pi_1$ unless $\pi = \pi_1$. Combining this with Lemma 4.3, the result follows from Theorem 3.2. ■

5 The Proof of Theorem 2.2

Denote by $\mathcal{R}(G)$ the *reduced graph* obtained from G by recursively deleting pendant vertices of the resultant graph until no pendant vertices remain. Let H be a subgraph of G and let N_H be the set of non-pendant vertices of H in G. Recall that $P_{d+1} = x_0 x_1 \dots x_d$ is a shortest path from x_0 to x_d. It is not hard to see that

$$d-1 \le |N_{P_{d+1}}| \le d+1. \tag{2}$$

Lemma 5.1 *If u and v are two vertices of $V\big(P_{d+1}\big) \cap V\big(\mathcal{R}(G)\big)$, then all the vertices of $V\big(P_{d+1}\big)$ between u and v belong to $V\big(\mathcal{R}(G)\big)$.*

Proof. Let u_0 and v_0 be two vertices of $V\big(P_{d+1}\big) \cap V\big(\mathcal{R}(G)\big)$ with maximum distance, that is, $dist\big(u_0, v_0\big) = \max\big\{dist(u,v) : \{u,v\} \subseteq V\big(\mathcal{R}(G)\big) \cap V\big(P_{d+1}\big)\big\}$. It suffices to show that all the vertices of $V\big(P_{d+1}\big)$ between u_0 and v_0 belong to $V\big(\mathcal{R}(G)\big)$. Suppose not, and let y be a vertex of $V\big(P_{d+1}\big)$ between u_0 and v_0 and $y \notin V\big(\mathcal{R}(G)\big)$. Then, there is a path $P_{u_0v_0}$ in $\mathcal{R}(G) \subseteq G - y$ connecting u_0 and v_0. Let x be the last vertex before y in P_{d+1} such that $x \in P_{u_0v_0}$, and let z be the first vertex after y in P_{d+1} such that $z \in P_{u_0v_0}$. In this case, there is another path P_{xz} connecting x and z such that $V\big(P_{xz}\big) \cap V\big(P_{u_0v_0}\big) = \{x, z\}$ and $y \in P_{xz}$, which means that x, y, z are in the same cycle of G, and thus $y \in V\big(\mathcal{R}(G)\big)$, a contradiction. ■

Corollary 5.2 *For any cycle C_g, at least $\lceil \frac{g}{2} \rceil - 1$ vertices of C_g are not on P_{d+1}.*

Proof. As $g > \lceil \frac{g}{2} \rceil$, the result holds for $|V(C_g) \cap V(P_{d+1})| \leq 1$. Thus, we may suppose that $|V(C_g) \cap V(P_{d+1})| \geq 2$. In this case, the distance of any two different vertices in C_g is at most $\lfloor \frac{g}{2} \rfloor$, so at most $\lfloor \frac{g}{2} \rfloor + 1$ vertices of C_g are contained in $V\big(P_{d+1}\big)$ by Lemma 5.1. Consequently, at least $g - \big(\lfloor \frac{g}{2} \rfloor + 1\big) = \lceil \frac{g}{2} \rceil - 1$ vertices of C_g are not on P_{d+1}. ■

Lemma 5.3 *If $G \in \mathbb{C}(n, d, p; c)$ and $c \geq 1$, then $p \leq n - d$, where the equality implies that x_0 and x_d are two pendant vertices of G, and either $g \in \{3, 4\}$ and $\mathcal{R}(G) = C_g$ with $|V\big(P_{d+1}\big) \cap V(C_g)| = g - 1$ or $\mathcal{R}(G) = B_1$ with $V\big(P_{d+1}\big) \cap V(B_1) = \big\{y_1, y_2, y_3\big\}$.*

Proof. Let C_g be an induced subgraph of G, as $c \geq 1$. By Corollary 5.2, there are at least $\lceil \frac{g}{2} \rceil - 1$ vertices of C_g that are not on P_{d+1}. Combining this with $g \geq 3$ and (2), it follows that

$$p \leq n - |N_{P_{d+1}}| - \Big(\Big\lceil \frac{g}{2} \Big\rceil - 1\Big) \leq n - \big(d-1\big) - \Big(\Big\lceil \frac{g}{2} \Big\rceil - 1\Big) = n - d + 2 - \Big\lceil \frac{g}{2} \Big\rceil \leq n - d, \quad (3)$$

as required.

We now suppose that $p = n - d$, that is, the equality holds in (3). In this case, P_{d+1} contains exactly $d - 1$ non-pendant vertices by (3), and so x_0 and x_d are two pendant vertices of G. Since P_{d+1} contains exactly $d - 1$ non-pendant vertices in G and since P_{d+1} cannot contain all vertices of C_g by Corollary 5.2, we conclude that $\mathcal{R}(G)$ contains exactly one vertex, say w_0, not on P_{d+1}, and we may suppose that $u_1u_2 \ldots u_{|V(\mathcal{R}(G))|-1}$ are the sub-path of P_{d+1} in $\mathcal{R}(G)$.

As P_{d+1} is a shortest path from x_0 to x_d, we have $N_G(u_1) \cap \big\{u_2, u_3, \ldots, u_{|V(\mathcal{R}(G))|-1}\big\} = \big\{u_2\big\}$ and $N_G\big(u_{|V(\mathcal{R}(G))|-1}\big) \cap \big\{u_1, u_2, \ldots, u_{|V(\mathcal{R}(G))|-2}\big\} = \big\{u_{|V(\mathcal{R}(G))|-2}\big\}$. Combining this with $\{u_1, u_{|V(\mathcal{R}(G))|-1}\} \subseteq V(\mathcal{R}(G))$, it follows that $w_0u_1 \in E(G)$ and $w_0u_{|V(\mathcal{R}(G))|-1} \in E(G)$. Now, since P_{d+1} is a shortest path from x_0 to x_d and since $u_1w_0u_{|V(\mathcal{R}(G))|-1}$ is a path of length two from u_1 to $u_{|V(\mathcal{R}(G))|-1}$, we have $|V(\mathcal{R}(G))| \in \{3,4\}$, as $w_0 \notin V(P_{d+1})$.

If $|V(\mathcal{R}(G))| = 3$, then $\mathcal{R}(G) = C_3$ and $|V(P_{d+1}) \cap V(C_3)| = 2$. Otherwise, $|V(\mathcal{R}(G))| = 4$.

If $u_2w_0 \in E(G)$, then $\mathcal{R}(G) = B_1$ and we may suppose that $V(P_{d+1}) \cap V(B_1) = \{y_1, y_2, y_3\}$ and $w_0 = y_4$. If $u_2w_0 \notin E(G)$, then $\mathcal{R}(G) = C_4$ and $|V(P_{d+1}) \cap V(C_4)| = 3$. ■

Lemma 5.4 *Suppose that $1 \le c \le 2$ and $2c \le d \le n-2$. (i) Let $G \in \mathbb{C}(n,d,n-d;c)$ with degree sequence π. If $\pi \ne \pi' = (n-d+1, 3^{(2c-1)}, 2^{(d-2c)}, 1^{(n-d)})$, then $\pi \lhd \pi'$. (ii) If $G \in \mathbb{C}(n,d,p;1)$ and $\pi \ne \pi_2$, then $\pi \lhd \pi_2$.*

Proof. We first prove (i). Since $p = n-d$ by $G \in \mathbb{C}(n,d,n-d;c)$, the degree sequence of G is equal to $\pi = (d_1, d_2, \ldots, d_d, 1^{(n-d)})$, where $d_1 \ge d_2 \ge \cdots \ge d_j \ge 3 > d_{j+1} = \cdots = d_d = 2$. By Lemma 5.3, x_0 and x_d are two pendant vertices of G and $j \ge 2c$. Note that $\pi \ne \pi'$, we have

$$\pi \unlhd (n-d+2c-j+1, 3^{(j-1)}, 2^{(d-j)}, 1^{(n-d)}) \lhd \pi',$$

and so (i) holds.

To prove (ii), if $p = n-d$, then (ii) follows from (i). If $p \le n-d-1$ and $c = 1$, then

$$\pi \unlhd (p+2, 2^{(n-p-1)}, 1^{(p)}) \unlhd (n-d+1, 2^{(d)}, 1^{(n-d-1)}) \lhd \pi_2,$$

completing the proof of (ii). ■

Lemma 5.5 *If $4 \le d \le n-2$, then*

$$\mathbb{U}(n,d) = \Big\{U_{1,1}(n,d), U_{1,2}(n,d), \ldots, U_{1,d-2}(n,d), U_{2,1}(n,d), U_{2,2}(n,d), \ldots, U_{2,d-3}(n,d)\Big\}.$$

Proof. It is not hard to see that $\{U_{1,1}(n,d), U_{1,2}(n,d), \ldots, U_{1,d-2}(n,d), U_{2,1}(n,d), U_{2,2}(n,d), \ldots, U_{2,d-3}(n,d)\} \subseteq \mathbb{U}(n,d)$. It suffices to show that $\mathbb{U}(n,d) \subseteq \{U_{1,1}(n,d), U_{1,2}(n,d), \ldots, U_{1,d-2}(n,d), U_{2,1}(n,d), U_{2,2}(n,d), \ldots, U_{2,d-3}(n,d)\}$. Let $U \in \mathbb{U}(n,d)$.

By Lemma 5.3, x_0 and x_d are two pendant vertices of U, so $|N_{P_{d+1}}| = d-1$. Besides, $g \in \{3,4\}$ and $|V(P_{d+1}) \cap V(C_g)| = g-1$. Let $z_1z_2\ldots z_{g-1}$ be the sub-path of P_{d+1} in

C_g. Since P_{d+1} is a shortest path from x_0 to x_d, $d(z_1) \geq 3$ and $d(z_{g-1}) \geq 3$. Since $d_3 = 2$ by the definition of π_2, we may suppose that $d(z_1) = n - d + 1$ and $d(z_{g-1}) = 3$.

In the case of $g = 3$, $z_1 z_2$ is the sub-path of P_{d+1} in C_3, $d(z_1) = n-d+1$ and $d(z_2) = 3$. Since x_0 and x_d are two pendant vertices of U, U is obtained from C_3 by attaching one path with j vertices together with $n-d-2$ isolated vertices to z_1, one path with $d-j-1$ vertices to z_2, where $1 \leq j \leq d-2$. Thus, $U = U_{1,j}(n,d)$ for some j, where $1 \leq j \leq d-2$. The case of $g = 4$ can be proceeded similarly and thus will be omitted here. ■

Proof of Theorem 2.2. In view of Theorems 3.3 and 3.4, it suffices to show that U has the maximum (resp., minimum) $H_f(U)$ if $f(x)$ is a strictly convex (resp., concave) function on $x \geq 1$. Let π be the degree sequence of U. If $\pi \neq \pi_2$, then $\pi \lhd \pi_2$ by Lemma 5.4. Combining this with Lemma 5.5, the result follows from Theorem 3.2. ■

6 The proof of Theorem 2.3

In what follows, if $c \geq 2$, then let $\mathcal{B}$ be a bicycle subgraph of $\mathcal{R}(G)$, and suppose that C_s and C_t are two cycles of $\mathcal{B}$ such that $|V(C_s) \cap V(C_t)| = r$. Furthermore, we always suppose that $V(C_s) \cap V(C_t) = \{w_0, w_1, \ldots, w_{r-1}\}$ when $r \geq 1$, and we define

$$dist\big(u_0', v_0'\big) = \max\big\{dist(u,v) : \{u,v\} \subseteq V(\mathcal{B}) \cap V\big(P_{d+1}\big)\big\}$$

when $|V(\mathcal{B}) \cap V\big(P_{d+1}\big)| \geq 2$.

Lemma 6.1 *Let $G \in \mathbb{C}(n,d,n-d-1;c)$ with degree sequence $(d_1, d_2, \ldots, d_n)$. If $c \geq 2$, then either $d_2 \geq 4$ or $d_3 \geq 3$. Furthermore, (i) If $r \geq 2$ and $|\{w_0, w_{r-1}\} \cap \{u_0', v_0'\}| = 2$, then $d_2 \geq 4$ and x_0 and x_d are two pendant vertices of G; (ii) If either $r \geq 2$ with $|\{w_0, w_{r-1}\} \cap \{u_0', v_0'\}| \leq 1$ or $r \leq 1$, then $d_3 \geq 3$.*

Proof. Since $G \in \mathbb{C}(n,d,n-d-1;c)$, G contains exactly $d+1$ non-pendant vertices. If $|V(\mathcal{B}) \cap V\big(P_{d+1}\big)| \leq 1$, note that $|N_{P_{d+1}}| \geq d-1$ by (2), then

$$|N_G| \geq |N_{P_{d+1}}| + |V(\mathcal{B})| - 1 \geq d - 1 + 3 = d + 2,$$

a contradiction. Therefore, $|V(\mathcal{B}) \cap V\big(P_{d+1}\big)| \geq 2$. Next, we consider three cases according to the value of r.

Case 1. $r \geq 2$.

In this case, we may suppose that $\mathcal{B} \cong B_{s_1,s_2,s_3}$, where $\min\{s_1, s_3\} \geq s_2 \geq 0$ and $\min\{s_1, s_3\} \geq 1$ (see Fig. 1). By the definition of r and the choices of u_0' and v_0', we have $r = s_2 + 2$, either $\{u_0', v_0'\} \subseteq V(C_{s_1+s_2+2})$, or $\{u_0', v_0'\} \subseteq V(C_{s_2+s_3+2})$ or $\{u_0', v_0'\} \subseteq V(C_{s_1+s_3+2})$.

Recall that $\mathcal{B}$ contains at least one vertex that is not on P_{d+1} by Corollary 5.2, and G contains exactly $d+1$ non-pendant vertices. Thus, $|N_{P_{d+1}}| \leq d$, and so $d-1 \leq |N_{P_{d+1}}| \leq d$ by (2).

We first suppose that $|N_{P_{d+1}}| = d-1$. Since P_{d+1} contains exactly $d-1$ non-pendant vertices of G and so x_0 and x_d are two pendant vertices of G, verifying that $\min\{d(u_0'), d(v_0')\} \geq 3$. If $\{u_0', v_0'\} = \{w_0, w_{s_2+1}\}$, then $d_1 \geq d_2 \geq \min\{d(u_0'), d(v_0')\} \geq 4$. Otherwise, $|\{w_0, w_{s_2+1}\} \cap \{u_0', v_0'\}| \leq 1$, then $d_1 \geq d_2 \geq d_3 \geq 3$, as required.

We secondly assume that $|N_{P_{d+1}}| = d$. That is, P_{d+1} contains exactly d non-pendant vertices of G. We claim that $\{u_0', v_0'\} \subseteq V(C_{s_1+s_3+2})$. Otherwise, by the symmetry of s_1 and s_3, we suppose that $\{u_0', v_0'\} \subseteq V(C_{s_1+s_2+2})$. Then $C_{s_1+s_2+2}$ contains at least $\lceil \frac{s_1+s_2}{2} \rceil$ vertices that are not on P_{d+1} by Corollary 5.2. Since G contains exactly $d+1$ non-pendant vertices and since each vertex of $\mathcal{B}$ is a non-pendant vertex, by (2) and $\min\{s_1, s_3\} \geq 1$, we have

$$d = |N_{P_{d+1}}| \leq d + 1 - \left\lceil \frac{s_1+s_2}{2} \right\rceil - s_3 \leq d + 1 - \left\lceil \frac{s_1+s_2}{2} \right\rceil - 1 \leq d - 1,$$

a contradiction. This completes our claim.

Since $\{u_0', v_0'\} \subseteq V(C_{s_1+s_3+2})$, $C_{s_1+s_3+2}$ contains at least $\lceil \frac{s_1+s_3}{2} \rceil$ vertices that are not on P_{d+1} by Corollary 5.2. Combining this with $|N_{P_{d+1}}| = d$ and $\min\{s_1, s_3\} \geq 1$, we have

$$d = |N_{P_{d+1}}| \leq d + 1 - \left\lceil \frac{s_1+s_3}{2} \right\rceil - s_2 \leq d + 1 - \left\lceil \frac{s_1+s_3}{2} \right\rceil \leq d,$$

and so $s_1 = s_3 = 1$ and $s_2 = 0$, that is, $\mathcal{B} \cong B_1$ with $y_2 = w_1$.

If $|\{u_0', v_0'\} \cap \{w_0, w_1\}| = 0$, then $\{u_0', v_0'\} = \{y_1, y_3\}$ (see Fig. 1). Note that $|N_{P_{d+1}}| = d$, then either $d(y_1) \geq 3$ or $d(y_3) \geq 3$, and hence $d_1 \geq d_2 \geq d_3 \geq 3$, as desired. Otherwise, $|\{u_0', v_0'\} \cap \{w_0, w_1\}| \geq 1$. We may suppose that $u_0' = w_0 = y_4$. In this case, $v_0' \in \{y_1, y_2, y_3\}$, and hence $|N_G| \geq |N_{P_{d+1}}| + |\{y_1, y_2, y_3\} \setminus \{v_0'\}| = d + 2$, a contradiction.

Case 2. $r = 1$.

In this case, $V(C_s) \cap V(C_t) = \{w_0\}$ and at least $\lceil \frac{s}{2} \rceil + \lceil \frac{t}{2} \rceil - 2$ vertices are not on P_{d+1} by Corollary 5.2. Combining this with (2), it follows that

$$d - 1 \leq |N_{P_{d+1}}| \leq d + 1 - \left(\left\lceil \frac{s}{2} \right\rceil + \left\lceil \frac{t}{2} \right\rceil - 2 \right) \leq d - 1, \tag{4}$$

and hence $|N_{P_{d+1}}| = d-1$. Thus, x_0 and x_d are two pendant vertices of G. If $w_0 \notin \{u_0', v_0'\}$, then $d_1 \geq d_2 \geq d_3 \geq 3$, as desired. Otherwise, u_0' and v_0' lie on the same cycle of $\mathcal{B}$. Without loss of generality, we suppose that $\{u_0', v_0'\} \subset V(C_t)$. By Corollary 5.2 and $|N_{P_{d+1}}| = d-1$ by (4), $|N_G| \geq |N_{P_{d+1}}| + s - 1 + \lceil \frac{t}{2} \rceil - 1 \geq d+2$, a contradiction.

Case 3. $r = 0$**.**

Since $\mathcal{B}$ is connected, there must be a path, say $P_k = u_1 u_2 \cdots u_k$, connecting C_s and C_t, where $u_1 \in V(C_s)$, $u_k \in V(C_t)$ and $k \geq 2$. Thus, $d(u_1) \geq 3$ and $d(u_k) \geq 3$.

By Corollary 5.2, at least $\lceil \frac{s}{2} \rceil + \lceil \frac{t}{2} \rceil - 2$ vertices are not on $V(P_{d+1})$. Similarly with (4), we have $|N_{P_{d+1}}| = d-1$ and hence x_0 and x_d are also two pendant vertices of G. If $|\{u_0', v_0'\} \cap \{u_1, u_k\}| \leq 1$, then $d_1 \geq d_2 \geq d_3 \geq 3$, as desired. Otherwise, $|\{u_0', v_0'\} \cap \{u_1, u_k\}| = 2$. Since $|N_{P_{d+1}}| = d-1$, and so $|N_G| \geq |N_{P_{d+1}}| + s - 1 + t - 1 \geq d+3$, a contradiction. ■

Lemma 6.2 *Let $B \in \mathbb{C}(n, d, p; 2)$. If $\pi \notin \{\pi_3, \pi_4\}$ and $4 \leq d \leq n-3$, then $\pi \lhd \pi_3$ or $\pi \lhd \pi_4$.*

Proof. Let $\pi = \left(d_1, d_2, \ldots, d_{n-p}, 1^{(p)}\right)$, where $d_1 \geq d_2 \geq \cdots \geq d_k \geq 4 > d_{k+1} = \cdots = d_j = 3 > d_{j+1} = \cdots = d_{n-p} = 2$. By Lemma 5.3, we have $p \leq n-d$. If $p = n-d$, then $\pi \lhd \pi_3$ by Lemma 5.4. Thus, we may assume that $p \leq n-d-1$ in the following, and we will prove that $\pi \lhd \pi_4$.

Case 1. $p = n-d-1$**.** By Lemma 6.1, $k \geq 2$ or $j \geq 3$.

If $k \geq 2$, since $\pi \neq \pi_4$ and $j \geq k \geq 2$,

$$\pi \unlhd \left(n-d-k-j+5, 4^{(k-1)}, 3^{(j-k)}, 2^{(d+1-j)}, 1^{(n-d-1)}\right) \lhd \pi_4.$$

Otherwise, $j \geq 3$. Since $\pi \neq \pi_4$, we have

$$\pi \unlhd \left(n-d-j+4, 3^{(j-1)}, 2^{(d+1-j)}, 1^{(n-d-1)}\right) \unlhd \left(n-d+1, 3^{(2)}, 2^{(d-2)}, 1^{(n-d-1)}\right) \lhd \pi_4.$$

Case 2. $p \leq n-d-2$**.** It is not hard to see that

$$\pi \unlhd \left(p-j+5, 3^{(j-1)}, 2^{(n-p-j)}, 1^{(p)}\right) \unlhd \left(n-d-j+3, 3^{(j-1)}, 2^{(d+2-j)}, 1^{(n-d-2)}\right). \quad (5)$$

Next, we prove that

$$\text{If } p = n-d-2, \quad \text{then} \quad j \geq 2. \quad (6)$$

Recall that C_s and C_t are two cycles of $\mathcal{B}$ such that $|V(C_s)\cap V(C_t)| = r$. We may suppose that $s \geq t \geq 3$. If $r \neq 1$, then $j \geq 2$ and hence (6) holds. Thus, we may assume that $r = 1$ in the following.

By contradiction, we assume that $j = 1$. Thus $\pi = \left(n-d+2, 2^{(d+1)}, 1^{(n-d-2)}\right)$. Let $V(C_s)\cap V(C_t) = \{w_0\}$. If $|V\left(P_{d+1}\right)\cap V(\mathcal{R}(B))| \leq 1$, then $|N_B| \geq |N_{P_{d+1}}|+s+t-2 \geq d+3$ by (2), a contradiction. Otherwise, $|V\left(P_{d+1}\right) \cap V(\mathcal{R}(B))| \geq 2$.

As in Lemma 5.1, let u_0 and v_0 be two vertices of $V\left(P_{d+1}\right) \cap V\left(\mathcal{R}(B)\right)$ with the maximum distance. Since $d_2 = 2$ and $d_1 = n-d+2$, B is obtained from $\mathcal{R}(B)$ by attaching $n-d-2$ paths to the 4-vertex of $\mathcal{R}(B)$. Combining this with $|V\left(P_{d+1}\right) \cap V(\mathcal{R}(B))| \geq 2$, we have $|\{u_0, v_0\} \cap \{x_0, x_d\}| \geq 1$ verifying that $|N_{P_{d+1}}| \geq d$.

If $w_0 \in \{u_0, v_0\}$, without loss of generality, we may assume that $w_0 = u_0$, and so $d(v_0) = 2$. In this case, $v_0 \in \{x_0, x_d\}$. Since $|N_{P_{d+1}}| \geq d$, by Corollary 5.2, we have $|N_B| \geq |N_{P_{d+1}}| + t - 1 + \lceil \frac{s}{2} \rceil - 1 \geq d+3$, a contradiction. Thus, $w_0 \notin \{u_0, v_0\}$.

Recall that B is obtained from $\mathcal{R}(B)$ by attaching $n-d-2$ paths to the 4-vertex of $\mathcal{R}(B)$ and $d_2 = 2$. Thus, $\left\{u_0, v_0\right\} = \left\{x_0, x_d\right\}$ and $|N_{P_{d+1}}| = d+1$. Again, Corollary 5.2 implies that $|N_B| \geq |N_{P_{d+1}}| + \left\lceil \frac{s}{2} \right\rceil - 1 + \left\lceil \frac{t}{2} \right\rceil - 1 \geq d+3$, a contradiction. This completes the proof of (6).

By combining (5) and (6), we have $\pi \trianglelefteq \left(n-d+1, 3, 2^{(d)}, 1^{(n-d-2)}\right) \triangleleft \pi_4$, as $\pi \neq \pi_4$. ■

Lemma 6.3 *If* $4 \leq d \leq n-3$, *then* $\mathbb{B}_1(n,d) = \left\{B_{1,i}(n,d), B_{2,j}(n,d),\right.$ *where* $1 \leq i \leq d-3$ *and* $\left.1 \leq j \leq \left\lfloor \frac{d}{2} \right\rfloor - 1\right\}$ *and* $\mathbb{B}_2(n,d) = \left\{B_{3,k}(n,d), B_{4,i}(n,d),\right.$ *where* $1 \leq i \leq d-3$ *and* $\left.1 \leq k \leq d-2\right\}$.

Proof. For $1 \leq i \leq d-3$, $1 \leq j \leq \left\lfloor \frac{d}{2} \right\rfloor - 1$ and $1 \leq k \leq d-2$, it is not hard to see that $B_{1,j} \in \mathbb{B}_1(n,d)$, $B_{2,j} \in \mathbb{B}_1(n,d)$, $B_{3,i} \in \mathbb{B}_2(n,d)$ and $B_{4,j} \in \mathbb{B}_2(n,d)$. Let B be a bicyclic graph of $\mathbb{B}_1(n,d) \cup \mathbb{B}_2(n,d)$.

Case 1. $B \in \mathbb{B}_1(n,d)$**.**

By Lemma 5.3, x_0 and x_d are two pendant vertices of B and $\mathcal{R}(B) = B_1$ with $V\left(P_{d+1}\right) \cap V(B_1) = \left\{y_1, y_2, y_3\right\}$ and so $\min\left\{d(y_1), d(y_2), d(y_3)\right\} \geq 3$. Since B contains exactly d non-pendant vertices by the definition of π_3, $\{x_1, x_2, \ldots, x_{d-1}, y_4\}$ are all these non-pendant vertices of B. Note that $\{y_1, y_2, y_3, y_4\}$ are the four vertices with degree at least three in B, and $d_1 = n-d+1 \geq 3 = d_2 = d_3 = d_4 > d_5$. Thus, y_1 is symmetric with y_3 and y_2 is symmetric with y_4, and either $d(y_1) = n-d+1$ or $d(y_2) = n-d+1$.

Here, we only consider the case of $d(y_2) = n-d+1$, as the case of $d(y_1) = n-d+1$ can be proved similarly. Since x_0 and x_d are two pendant vertices of B and since $d(y_2) = n-d+1$, B is obtained from B_1 by attaching $n-d-2$ isolated vertices to y_2, one path with q vertices to y_1, and another path with $d-q-2$ vertices to y_3, where $1 \le q \le d-3$. It is easily checked that $B_{2,q}(n,d) = B_{2,d-2-q}$, and so $B = B_{2,j}$, where $1 \le j \le \lfloor \frac{d}{2} \rfloor - 1$.

Case 2. $B \in \mathbb{B}_2(n,d)$**.**

Recall that C_s and C_t are two cycles of $\mathcal{B}$ with $|V(C_s) \cap V(C_t)| = r$. By Lemma 6.1, $r \ge 2$ and hence we may suppose that $V(C_s) \cap V(C_t) = \{w_0, w_1, \ldots, w_{r-1}\}$, $s \ge t \ge 2(r-1)$ and $\min\{d(w_0), d(w_{r-1})\} = 4$, as x_0 and x_d are two pendant vertices of G and $\{w_0, w_{r-1}\} = \{u_0', v_0'\}$ (see Lemma 6.1). Since $\{w_0, w_{r-1}\} = \{u_0', v_0'\}$ and $s \ge t \ge 2(r-1)$, at least $s+t-2r$ vertices of $V(\mathcal{R}(B))$ are not on P_{d+1}. Combining this with (2),

$$d-1+(s+t-2r) \le |N_{P_{d+1}}| + (s+t-2r) \le |N_B| = d+1, \tag{7}$$

and hence $2(r-1) \le t \le r+1$. Thus, $2 \le r \le 3$.

Combining with $t \ge 3$, we have $t = r+1$. By (7) and $s \ge t = r+1$, we have $d+1 = |N_B| \ge d-1+2(r+1)-2r = d+1$, which implies that $s = t = r+1$. Recall that $|V(C_s) \cap V(C_t)| = r \in \{2,3\}$. Thus, $\mathcal{R}(B) \in \{B_1, B_2\}$. In view of the definition of π_4 and since $\min\{d(w_0), d(w_{r-1})\} = 4$, we may suppose that $d(w_0) = n-d+1$.

We first suppose that $\mathcal{R}(B) = B_1$ and we may assume that $y_2 = w_0$ by symmetry. Since x_0 and x_d are two pendant vertices of B, B is obtained from B_1 by attaching one path with k vertices together with $n-d-3$ isolated vertices to y_2, and one path with $d-k-1$ vertices to y_4, where $1 \le k \le d-2$, this implying that $B = B_{3,k}(n,d)$ for some $1 \le k \le d-2$. Now, we suppose that $\mathcal{R}(B) = B_2$. In a similar way, we can conclude that $B = B_{4,i}(n,d)$ for $1 \le i \le d-3$, and so complete the proof of this result. ■

Proof of Theorem 2.3. In view of Theorems 3.3 and 3.4, it suffices to show that B has the maximum (resp., minimum) $H_f(B)$ if $f(x)$ is a strictly convex (resp., concave) function on $x \ge 1$. Suppose that the degree sequence of B is π. If $\pi \in \{\pi_3, \pi_4\}$, then Lemma 6.3 implies that $B \in \mathbb{B}_1(n,d) \cup \mathbb{B}_2(n,d)$. Otherwise, $\pi \notin \{\pi_3, \pi_4\}$. Since $4 \le d \le n-3$, $\pi \lhd \pi_3$ or $\pi \lhd \pi_4$ by Lemma 6.2. Now, the result follows from Theorem 3.2. ■

Remark 6.4 Actually, in this paper, we have determined all the extremal graphs with maximum (resp., minimum) vertex-degree-function index $H_f(G)$ for any strictly convex (resp., concave) function $f(x)$ defined on $x \geq 1$ among the class of trees, unicyclic graphs and bicyclic graphs with given diameter, respectively.

Acknowledgment. The authors are grateful to the anonymous referee for helpful suggestions and valuable comments, which led to an improvement of the original manuscript. This paper is partially supported by NNSF of China (No. 11571123), Training Program for Outstanding Young Teachers in University of Guangdong Province (No. YQ2015027), Guangdong Province Ordinary University Characteristic Innovation Project (No. 2017K-TSCX020), and a grant from the Simons Foundation (522728, XG).

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