MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **86** (2021) 17-28

ISSN 0340 - 6253

Extremal Zagreb Indices of Graphs of Order n with p Pendent Vertices

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(Received October 18, 2020)

Abstract

The first and the second Zagreb indices of a connected graph are defined as the sum of squares of its vertex degrees, and the sum of the products of degrees of adjacent vertices, respectively. In this paper, we determine the graphs with maximum Zagreb indices and the minimum first Zagreb index in ζ_n^p, the class of all connected graphs of order n with p pendent vertices, where $0 \leq p \leq n-1$. Also, we determine the graphs with minimum second Zagreb index in ζ_n^p, for $p = \{0, 1, 2, 3, 4, n-3, n-2, n-1\}$.

1 Introduction

All graphs in this paper are assumed to be simple, connected and finite. Let $G = (V, E)$ be a graph, with the vertex set $V = V(G)$ and the edge set $E = E(G)$. In theoretical chemistry, the physico-chemical properties of chemical compounds are often modeled by using molecular-graph-based structure descriptors, and are referred to as topological indices [12, 20].

The first and the second Zagreb indices of a graph G, denoted by $M_1(G)$ and $M_2(G)$, respectively, have been introduced almost fifty years ago. by Gutman and Trinajestić [13].

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They are defined as

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

where $d(v)$ (also denoted by $d_G(v)$) is the degree of vertex $v \in V$, which is the number of edges incident v. The extent of branching of the molecular carbon-atom skeleton can be calculated by M_1 and M_2, so they used as molecular descriptors [2, 19]. Various classes of graphs have been investigated to finding graphs with maximum and minimum Zagreb indices. For instance, extremal values of Zagreb indices are determined in the classes of graphs with a given number of cut edges, clique number, and vertex connectivity at most k, in [5], [22], and [16], respectively. In [4], extremal values of Zagreb indices are determined in the class of trees with a given number of vertices of maximum degree. Gutman and Kamran Jamil and Akhter characterized graphs with n vertices, p pendent vertices, with positive cyclomatic number (= the number of independent cycles), and minimal M_1 [11]. Also, Li and Zhang studied sharp upper bounds for Zagreb indices of bipartite graphs with a given diameter [15]. Furthermore Feng and Ilić presented sharp bounds for the Zagreb indices of graphs with a given matching number [7]. Li, Yang and Zhao determined sharp upper and lower bounds of the cacti with p pendent vertices for Zagreb indices [14]. Also Goubko [8, 9], determined sharp lower bounds of Zagreb indices for trees and chemical trees with a given number of pendent vertices and found optimal trees. Furthermore, Goubko and Gutman in [10], offer a dynamic programming method that characterizes the trees with a given number of pendent vertices, for which a vertex-degree-based invariant (topological index) achieves its extremal value. For more details of Zagreb indices, we refer to [3, 18].

Note that the results of Goubko [8] are obtained for a certain number of pendent vertices, but not for a fixed order of the graphs. In this paper, we determine the maximum Zagreb indices and the minimum first Zagreb index of graphs of order n, with p pendent vertices.

We follow the standard graph-theoretic terminology. Let $G = (V, E)$ be a simple graph and $v \in V$ be a vertex of G. We denote the set of neighbors of v by $N_G(v)$. Also we put $N_G[v] = N_G(v) \cup \{v\}$. Note that $d(v) = |N_G(v)|$. If $V = \{v_1, \ldots, v_n\}$ and $d(v_i) = d_i$, the sequence $(d_1, d_2, \ldots, d_n)$ is called a degree sequence of G. We say that two graphs G and

H are isomorphic and write $G \cong H$, if there is a bijection $f : V(G) \longrightarrow V(H)$ such that $uv \in E(G)$ if and only if $f(u)f(v) \in E(H)$ [21]. If $u, v \in V(G)$ and $\{v_1, v_2, \ldots, v_i\}$ is a subset of $N_G(v) \setminus N_G[u]$, we put

$$G^* = G - \sum_{v_i \in N_G(v)} vv_i + \sum_{v_i \in N_G(v)} uv_i \ .$$

In [24], the process of obtaining G^* from G is called a graft transformation.

We denote the maximum degree of vertices in G by Δ or $\Delta(G)$. We denote the path with n vertices, the complete graph with n vertices and the star graph with $n+1$ vertices by P_n, K_n and S_n, respectively. A clique in a graph is a set of pairwise adjacent vertices. The length of a shortest cycle in graph G is called the girth of G. Recall that a unicyclic graph is a connected graph containing exactly one cycle. We denote by F_n^k the unicyclic graph obtained by attaching a path of length $n-k$ to the cycle C_k of length k.

The Dumbbell graph $D(n; s, t)$ consists of a path with $n-s-t$ vertices, with s pendent vertices adjacent to one of the end vertex of the path P_{n-s-t} and t pendent vertices adjacent to the other end vertex of the path P_{n-s-t}. We denote the graph obtained from adjoining one vertex of complete graph K_{n-p} to p pendent vertices by K_{n-p}^p.

Let χ_n^p be the class of all trees of order n with p pendent vertices. Suppose $T \in \chi_n^p$. It is well-know [21] that every tree with maximum degree $\Delta > 1$ has at least Δ vertices of degree 1. Also is obvious that if n_i is the number of the vertices of degree i , $1 \leq i \leq n$, in T, then $\sum_{i=1}^{p} in_i = 2(n-1)$ and $\sum_{i=1}^{p} n_i = n$. Therefore

$$\sum_{i=3}^{p} (i-2)n_i = p - 2. \tag{1}$$

Let ζ_n^p be the class of all connected graphs of order n with p pendent vertices, where $0 \leq p \leq n-1$. It is clear that $\zeta_1^0 = \zeta_2^0 = \zeta_2^1 = \zeta_3^1 = \emptyset$, also the classes ζ_2^2, ζ_3^0 and ζ_n^{n-1}, respectively contain the unique graphs P_2, K_3 and star graph S_{n-1}. So in order to find the graphs with maximum or minimum Zagreb indices in ζ_n^p, we may assume that $0 \leq p \leq n-2$, and $n \geq 4$.

In section 2, we state and prove some results, which are useful in proving the main results of the paper. In Section 3 we show that $D(n; n-3, 1)$ and K_{n-p}^p have maximum Zagreb indices in ζ_n^{n-2} and ζ_n^p $(p \neq n-2)$, respectively. We prove that C_n and F_n^k have minimum Zagreb indices in ζ_n^0 and ζ_n^1, respectively. Also, we determine degree sequence of trees which have minimum first Zagreb index in ζ_n^p, $2 \leq p \leq n-2$, and we prove that $D(n; \lceil \frac{p}{2} \rceil, \lfloor \frac{p}{2} \rfloor)$ has minimum second Zagreb index in ζ_n^p, $p \in \{2, 3, 4, n-3, n-2\}$.

2 Prerequisites

In this section we state some known results and prove some results that will be used in the next sections. We begin with the following proposition which is proved by Aghel et.al.

Proposition 2.1. *[1, Lemma 3.1] Let $G = (V, E)$ is a simple connected graph, and $u, v \in V(G)$, for $i = 1, 2$ we have*

(i) If $uv \notin E(G)$, then $M_i(G) < M_i(G + uv)$.

(ii) If $uv \in E(G)$, then $M_i(G) > M_i(G - uv)$.

A caterpillar is a tree in which all the vertices are within distance 1 of a central path.

Lemma 2.2. *[17, Lemma 3] Suppose that T is a tree of order n, which is non-caterpillar. Then there exists a caterpillar T' of order n such that T' and T have the same degree sequence.*

Theorem 2.3. *[6, Theorem 5.2] Let G be a unicyclic graph of order n and girth k, which is different from C_n. If $G \ncong F_n^k$, then $M_i(F_n^k) < M_i(G)$, $i = 1, 2$.*

Lemma 2.4. *[6, Lemma 4.1] Let w be a vertex of connected graph $G \neq P_1$ and $k, l \geq 1$. Let G_1 be the graph obtained from G by attaching pendent paths $P' = wv_1v_2 \dots v_k$ and $P'' = wu_1u_2 \dots u_l$, and let G_2 be the graph obtained from the same graph G by attaching a path $P^* = wv_1v_2 \dots v_ku_1u_2 \dots u_l$ (see Figure 1). Then $M_i(G_2) < M_i(G_1)$.*

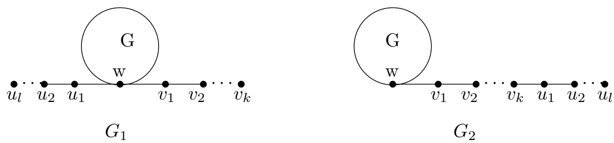

Figure 1

Theorem 2.5. *[23, 25] The cycle C_n is the unique graph with minimum Zagreb indices M_i, $i = 1, 2$, among all unicyclic graphs with n vertices.*

The next Lemma is proved in [6]. But there are some miscalculations in lines 4, 6, 8, 10, and 12 on page 601. In that proof for the case (ii), in calculating $M_2(G)$, $M_2(G')$, and $M_2(G'')$, the value $d(u)d(v)$ has subtracted from each relation. Because they mistakenly assumed that due to the adjacency of vertices u and v, this value was calculated twice.

Also, because of these miscalculations in $M_2(G)$, $M_2(G')$, and $M_2(G'')$, the values Δ_1 and Δ_2 are not correct. We re-prove this case:

Lemma 2.6. *[6, Lemma 2.2]. Let u and v be the two vertices in a graph G. Let $u_1, u_2, \ldots, u_r$ be pendent vertices adjacent to u, and $v_1, v_2, \ldots, v_t$ be pendent vertices adjacent to v (r, t are not necessarily the total number of pendent vertices adjacent to u and v). Let $G' = G - \{uu_1, uu_2, \ldots, uu_r\} + \{vu_1, vu_2, \ldots, vu_r\}$, $G'' = G - \{vv_1, vv_2, \ldots, vv_t\} + \{uv_1, uv_2, \ldots, uv_t\}$ (see Figure 2). Then at least one of inequalities $M_i(G) < M_i(G')$ or $M_i(G) < M_i(G'')$, $i = 1, 2$, is valid.*

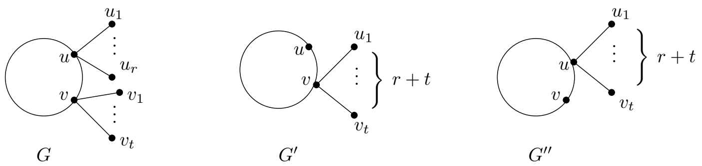

Figure 2

Proof. According to discussion preceding Lemma, we consider only the second Zagreb index, in case that the vertices u and v are adjacent. Put $G_0 = G - \{u_1, u_2, \ldots, u_r, v_1, v_2, \ldots, v_t\}$, and let $d_{G_0}(u) = p, d_{G_0}(v) = q$. If $uv \in E(G_0)$, then $u \in N_{G_0}(v)$ and $v \in N_{G_0}(u)$. We calculate $M_2(G)$, $M_2(G')$ and $M_2(G'')$ as follows

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

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

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

Now we have

$$\Delta_1 = M_2(G') - M_2(G) = r\Big(\sum_{x\in N_{G_0}(v)-\{u\}} d_{G_0}(x) - \sum_{x\in N_{G_0}(u)-\{v\}} d_{G_0}(x)\Big) + rt.$$

$$\Delta_2 = M_2(G'') - M_2(G) = t\Big(\sum_{x\in N_{G_0}(u)-\{v\}} d_{G_0}(x) - \sum_{x\in N_{G_0}(v)-\{u\}} d_{G_0}(x)\Big) + rt.$$

If $\Delta_1 \le 0$, then $\sum_{x\in N_{G_0}(u)-\{v\}} - \sum_{x\in N_{G_0}(v)-\{u\}} \ge t$. Since $r, t \ge 1$ we have

$$\Delta_2 = t\Big(\sum_{x\in N_{G_0}(u)-\{v\}} d_{G_0}(x) - \sum_{x\in N_{G_0}(v)-\{u\}} d_{G_0}(x)\Big) + rt \ge tr + t^2 > 0.$$

Also If $\Delta_2 \le 0$, then $\sum_{x\in N_{G_0}(v)-\{u\}} - \sum_{x\in N_{G_0}(u)-\{v\}} \ge r$. Since $r, t \ge 1$ we have

$$\Delta_1 = r\Big(\sum_{x\in N_{G_0}(v)-\{u\}} d_{G_0}(x) - \sum_{x\in N_{G_0}(u)-\{v\}} d_{G_0}(x)\Big) + rt \ge rt + r^2 > 0.$$

Thus the result follows. ■

Corollary 2.7. *In the class of dumbbell graphs of order n with p pendent vertices, $D(n; 1, p-1)$ has the maximum first and second Zagreb indices, and $D(n; \lceil \frac{p}{2} \rceil, \lfloor \frac{p}{2} \rfloor)$, has the minimum first and second Zagreb indices.*

Theorem 2.8. *Let κ_n^p be the class of all caterpillars of order n with p pendent vertices. Then for $n \ge 4$, and $2 \le p \le n-2$, the caterpillars in κ_n^p with a degree sequence π have a minimum first Zagreb index, where*

$$\pi = (\underbrace{\Delta, \ldots, \Delta}_{n_\Delta}, \underbrace{\Delta-1, \ldots, \Delta-1}_{n-n_\Delta-p}, \underbrace{1, \ldots, 1}_{p}),$$

and

$$\Delta = \left\lceil \frac{p-2}{n-p} \right\rceil + 2, \qquad n_\Delta = p(\Delta-2) - n(\Delta-3) - 2.$$

Proof. Let $T \in \kappa_n^p$. By repeating use of Lemma 2.6 we obtain a caterpillar T' in κ_n^p such that $M_1(T') \le M_1(T)$ and the difference between the degrees of both non-pendent vertices in T' is at most one. Therefore T has vertices of degrees Δ, $\Delta - 1$ and 1; hence $\Delta = \lceil \frac{p-2}{n-p} \rceil + 2$.

Suppose n_Δ and $n_{\Delta-1}$ be the numbers of vertices in the T', with degrees Δ and $\Delta - 1$, respectively. By (1), we have

$$n_\Delta(\Delta-2) + n_{\Delta-1}(\Delta-3) = p-2. \tag{2}$$

Adding $p(\Delta-3)$ to both sides of (2), we obtain that

$$(\Delta-3)(n_\Delta+n_{\Delta-1}+p)+n_\Delta=p(\Delta-2)-2.$$

Since $n_\Delta+n_{\Delta-1}+p=n$, we have $n_\Delta=p(\Delta-2)-n(\Delta-3)-2$. ■

Lemma 2.9. *Suppose that T is a tree of order n. Let $\{u,v,w,x,y,z\}\subset V(T)$ and $\{uv,vw,xy,yz\}\subset E(T)$, where $d(u)=1$. Let*

$$T'=T-\{uv,vw,xy,yz\}+\{uy,yw,xv,vz\}.$$

Then $M_2(T')<M_2(T)$ if one of the following conditions holds

(i) $d(y)>d(v)$ and $d(x)+d(z)>d(u)+d(w)$.

(ii) $d(y)<d(v)$ and $d(x)+d(z)<d(u)+d(w)$.

Proof. Since

$$M_2(T)-M_2(T')=(d(y)-d(v))(d(z)+d(x)-d(w)-1),$$

the result is clear. ■

Lemma 2.10. *Let T and T' be trees of order n with p pendent vertices which are not the dumbbell graphs. Suppose that T and T' have exactly one vertex of degree more than 2 and exactly two vertices of degree more than 2, respectively; and the other non-pendent vertices have degree 2. Then we have*

(i) $M_2(D(n;\lceil\frac{p}{2}\rceil,\lfloor\frac{p}{2}\rfloor)<M_2(T)$.

(ii) $M_2(D(n;\lceil\frac{p}{2}\rceil,\lfloor\frac{p}{2}\rfloor)<M_2(T')$.

Proof. (i) By the definition of T, there exists a vertex $v\in V(T)$ with $d(v)\geq 3$. Since T is not a dumbbell graph, there exists a path $a_m a_{m-1}\dots a_1 v b_1\dots b_{l-1}b_l$, such that $m,l\geq 2$, $d(b_l)=d(a_m)=1$. Put

$$T_1=T-\{a_1v,b_1v,b_{l-1}b_{l-2},b_{l-1}b_l\}+\{a_1b_{l-1},b_1b_{l-1},vb_{l-2},vb_l\}.$$

Since $d(v)\geq 3$, by Lemma 2.9, $d(b_l)=1$ and the other non-pendent vertices have degree 2. Hence $M_2(T_1)<M_2(T)$. We repeat this graft transformation until we get a tree T^*, such

that a vertex v in T^* is adjacent to $p-1$ pendent vertices, and hence $T^* \cong D(n; p-1, 1)$. Thus we have

$$M_2(D(n; p-1, 1)) < \cdots < M_2(T_1) < M_2(T),$$

and by Corollary 2.7 we obtain that

$$M_2(D(n; \lceil \frac{p}{2} \rceil, \lfloor \frac{p}{2} \rfloor)) \leq M_2(D(n; p-1, 1)) < M_2(T).$$

(ii) Let $\{u, v\} \subset V(T')$, $d(u) = r \geq 3$, $d(v) = s \geq 3$. We repeatedly use the graft transformation expressed in Lemma 2.9, on the vertices u and v, until we get $D(n; r-1, s-1)$. Since T' is not a dumbbell graph, $M_2(D(n; r-1, s-1)) < M_2(T')$. By Corollary 2.7 we have

$$M_2(D(n; \lceil \frac{p}{2} \rceil, \lfloor \frac{p}{2} \rfloor)) \leq M_2(D(n; r-1, s-1)) < M_2(T'),$$

and the result follows. ■

3 Graphs with maximum and minimum Zagreb indices in ζ_n^p

Theorem 3.1. *Let G_1^* and G_2^* have maximum Zagreb indices M_1 and M_2, respectively, in ζ_n^p, where $n \geq 4$ and $0 \leq p \leq n-2$. Then*

(i) If $p = n-2$, then $G_1^* \cong G_2^* \cong D(n; n-3, 1)$.

(ii) If $p \neq n-2$, then $G_1^* \cong G_2^* \cong K_{n-p}^p$.

Proof. (i) In this case we know that the class ζ_n^{n-2} contains only $D(n; r, t)$, where $r + t = n-2$. According to Corollary 2.7, for $2 \leq r \leq t$, we have $M_i(D(n; r, t)) < M_i(D(n; n-3, 1))$, $i = 1, 2$. So $G_1^* \cong G_2^* \cong D(n; n-3, 1)$.

(ii) If $p = 0$, then it is clear that $G_1^* \cong G_2^* \cong K_n$. Thus suppose that $p \neq 0, n-2$ and let $G_1 \in \zeta_n^p$. We partition $V(G_1)$ into $A \cup B$, where $A = \{v \in G_1 \mid d(v) = 1\}$ and $B = \{v \in G_1 \mid d(v) \geq 2\}$. If $u, v \in B, uv \notin E(G_1)$, then by adding an edge between u and v, we have $M_i(G_1 + uv) > M_i(G_1)$, $i = 1, 2$. We continue this process on B, until all vertices in B become adjacent to each other. In this way we get a graph G_2, with a clique K_{n-p} of order $n-p$. If all vertices in A, are not adjacent to one vertex of the K_{n-p}, then we apply Lemma 2.6 on G_2, so that we get K_{n-p}^p, which has maximum Zagreb indices in this class. ■

Theorem 3.2. *Let G_1^* and G_2^* be the graphs in ζ_n^0, with minimum Zagreb indices M_1 and M_2, respectively, where $n \geq 4$. Then $G_1^* \cong G_2^* \cong C_n$.*

Proof. Let $G \ncong C_n$ and $G \in \zeta_n^0$. Then G has at least one cycle. If G is unicyclic, then by Lemma 2.5 we have $M_i(C_n) < M_i(G)$. If G has more than one cycle, then by removing edges along some cycles of G, we get a unicyclic spanning subgraph G_1, such that $M_i(G_1) < M_i(G)$, and by Theorem 2.5 the result follows. ■

Theorem 3.3. *Let G_1^* and G_2^* have minimum Zagreb indices M_1 and M_2, respectively in ζ_n^1, where $n \geq 4$. Then there exsits $3 \leq k \leq n-1$ so that, $G_1^* \cong F_n^k$ and $G_2^* \cong F_n^{n-1}$.*

Proof. Suppose that $G \in \zeta_n^1$. Since G has exactly one pendent vertex, G has at least one cycle. Therefore G has a unicyclic spanning subgraph G_1. It is clear that $M_i(G_1) \leq M_i(G)$, and according to Theorem 2.3, we have $M_i(F_n^k) \leq M_i(G_1)$, $i = 1, 2$. Also it is easy to see that

$$\begin{cases} M_1(F_n^k) = 4n + 2 & \text{if } \ 3 \leq k \leq n-1, \\ M_2(F_n^k) = 4n + 4 & \text{if } \ 3 \leq k \leq n-2, \\ M_2(F_n^{n-1}) = 4n + 3 & \text{if } \ k = n-1. \end{cases}$$

The above relations yield that if G_1^* in ζ_n^1 has minimum first Zagreb index, then there exists $3 \leq k \leq n-1$ such that $G_1^* \cong F_n^k$. In this case G_1^* is not unique. Also if G_2^* has minimum second Zagreb index in ζ_n^1, then $G_2^* \cong F_n^{n-1}$. ■

Let $G \in \zeta_n^p$, where $2 \leq p \leq n-2$, and suppose that G is not a tree. Suppose that T is a spanning tree of G. We know that $M_i(T) < M_i(G)$. By removing edges from G to get a spanning tree, the number of pendent vertices may increase. In this case choose a vertex v, which is adjacent to at least two pendent paths and $d(v) \geq 3$. By applying Lemma 2.4, we convert these pendent paths to one pendent path. This graft transformation, decreases the number of pendent vertices and the Zagreb indices. We repeat this transformation, until we get a tree T' with p pendent vertices, such that $M_i(T') \leq M_i(T) < M_i(G)$. So to determine the graphs with minimum Zagreb indices, we investigate the class χ_n^p instead of the class ζ_n^p.

The following Theorem has been proved by Gutman and Kamran Jamil [11, Theorem 4.1]. We prove it in a different way, using the degree sequences of caterpillars with the minimum first Zagreb index.

Theorem 3.4. *Let the tree T^* has minimum first Zagreb index in χ_n^p, where $n \geq 4$ and $2 \leq p \leq n-2$. Then T^* is isomorphism to the tree T with degree sequence π, where*

$$\pi = (\underbrace{\Delta, \ldots, \Delta}_{n_\Delta}, \underbrace{\Delta-1, \ldots, \Delta-1}_{n-n_\Delta-p}, \underbrace{1, \ldots, 1}_{p}),$$

and

$$\Delta = \left\lceil \frac{p-2}{n-p} \right\rceil + 2, \qquad n_\Delta = p(\Delta-2) - n(\Delta-3) - 2.$$

Proof. Note that the value of M_1 is dependent only on the degree of each vertex and is independent of the degree of the neighbors of the vertices. Hence if we determine the vertex degree sequence of the tree which has a minimum M_1, then any graph with this degree sequence has a minimum M_1. By Lemma 2.2, for all $T \in \chi_n^p$, there exists $T' \in \kappa_n^p$ so that T and T' have same degree sequence. Also, according to Theorem 2.8 all caterpillar with the degree sequence $(\underbrace{\Delta, \ldots, \Delta}_{n_\Delta}, \underbrace{\Delta-1, \ldots, \Delta-1}_{n-n_\Delta-p}, \underbrace{1, \ldots, 1}_{p})$ have a minimum first Zagreb index in κ_n^p. Thus the result follows. ■

Theorem 3.5. *Let T^* is a tree in χ_n^p with minimum second Zagreb index. Then for $n \geq 4$, and $p \in \{2, 3, 4, n-3, n-2\}$, we have $T^* \cong D(n; \lceil \frac{p}{2} \rceil, \lfloor \frac{p}{2} \rfloor)$.*

Proof. If $p = 2$ we let $T \in \chi_n^2$. It is clear that there is no vertex of degree more than 2 in T. So there are exactly $n-2$ vertices of degree 2 and 2 vertices of degree 1 in T. Therefore χ_n^2 contains a unique tree P_n. Thus we have $T^* \cong P_n \cong D(n; 1, 1)$.

If $p = 3$, then it follows from (1) that $n_3 = 1$. So χ_n^3 contains only the trees with the degree sequence π, where

$$\pi = (3, \underbrace{2, \ldots, 2}_{n-p-1}, \underbrace{1, \ldots, 1}_{p}).$$

Hence by Lemma 2.10, $T^* \cong D(n; 2, 1)$.

If $p = 4$, then it follows from (1) that $n_3 + 2n_4 = 2$. So χ_n^4 contains only the trees with the degree sequences π and π', where

$$\pi = (4, \underbrace{2, \ldots, 2}_{n-p-1}, \underbrace{1, \ldots, 1}_{p}), \qquad \pi' = (3, 3, \underbrace{2, \ldots, 2}_{n-p-2}, \underbrace{1, \ldots, 1}_{p}).$$

Thus by Lemma 2.10, $T^* \cong D(n; 2, 2)$.

If $p = n-2$, we know that χ_n^{n-2} contains exactly $D(n; r, t)$, where $r + t = n-2$. According to the Corollary 2.7, we have $T^* \cong D(n; \lceil \frac{p}{2} \rceil, \lfloor \frac{p}{2} \rfloor)$.

If $p = n-3$, then it is clear that χ_n^{n-3} contains only caterpillar graphs. Let $T_1 \in \chi_n^{n-3}$, which is not dumbbell graph and $t \geq r$ (see Figure 3) and

$$T_2 = T_1 - \{vv_1, \ldots, vv_s\} + \{uv_1, \ldots, uv_s\}.$$

Then $T_2 \cong D(n; r+s, t)$, and we have

$$M_2(T_1) - M_2(T_2) = s(t - r + 1).$$

Since $t \geq r$ and $s \geq 1$, $M_2(T_2) < M_2(T_1)$. Also by Lemma 2.7, $D(n; \lceil \frac{p}{2} \rceil, \lfloor \frac{p}{2} \rfloor) \leq D(n; r+s, t)$. The equality hold if and only if $D(n; \lceil \frac{p}{2} \rceil, \lfloor \frac{p}{2} \rfloor) \cong D(n; r+s, t)$. ■

Figure 3

Acknowledgment: The authors gratefully thank the four anonymous referees for the constructive comments and recommendations which definitely help to improve the readability and quality of the paper.

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