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On Zagreb Eccentricity Indices of Trees

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Abstract

For a connected graph, the first Zagreb eccentricity index is defined as the sum of the squares of the eccentricities of the vertices, and the second Zagreb eccentricity index is defined as the sum of the products of the eccentricities of pairs of adjacent vertices. We determine the trees with minimum Zagreb eccentricity indices when domination number, maximum degree, and bipartition size are respectively given, and we also discuss the trees with maximum Zagreb eccentricity indices when domination number is given.

1 Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, $deg_G(u)$ or $deg(u)$ denotes the degree of u in G. For $u \in V(G)$, $e_G(u)$ or $e(u)$ denotes the eccentricity of u in G, which is equal to the largest distance from u to other vertices.

The Zagreb indices have been introduced more than forty years ago by Gutman and Trinajstić [10, 11], which are the most known and widely studied topological indices [3, 9, 13, 23, 24, 26]. The first Zagreb index of G is defined as

$$M_1(G) = \sum_{u \in V(G)} deg^2(u),$$

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while the second Zagreb index of G is defined as

$$M_2(G) = \sum_{uv \in E(G)} deg(u)deg(v).$$

It should be pointed out that the Zagreb indices and their variants are useful molecular descriptors which found considerable use in QSPR and QSAR studies as summarized by Todeschini and Consonni [18, 19]. Several graph invariants based on vertex eccentricities attract some attention in chemistry and subject to large number of studies. In an analogy with the first and the second Zagreb indices, Vukičevic and Graovac [20] and Ghorbani and Hosseinzadeh [8] introduced two types of Zagreb eccentricity indices by replacing degrees by eccentricity of the vertices. Thus the first Zagreb eccentricity index of G is defined as

$$\xi_1(G) = \sum_{u \in V(G)} e^2(u),$$

while the second Zagreb eccentricity index of G is defined as

$$\xi_2(G) = \sum_{uv \in E(G)} e(u)e(v).$$

Some mathematical and computational properties of the Zagreb eccentricity indices have been obtained in [4, 21]. Among them, various lower and upper bounds for the Zagreb eccentricity indices were given, the n-vertex trees with the first a few smallest and largest Zagreb eccentricity indices for $n \geq 6$ were determined, the trees with minimum and maximum Zagreb eccentricity indices were determined when diameter, number of pendent vertices, and matching number are respectively given, and the trees with maximum Zagreb eccentricity indices when maximum degree is given. [2] presented some properties, upper and lower bounds of the Zagreb eccentricity indices and also characterized the extremal graphs. [12] computed the generalized hierarchical product of the Zagreb eccentricity indices.

In this paper, we determine the trees with minimum Zagreb eccentricity indices when domination number, maximum degree, and bipartition size are respectively given, and we also determine the trees with maximum Zagreb eccentricity indices when domination number $\gamma = 2, \lceil \frac{n}{3} \rceil, \frac{n}{2}$.

For $u, v \in V(G)$, $d_G(u, v)$ or $d(u, v)$ denotes the distance between u and v in G. Let S_n, P_n, C_n and K_n be the n-vertex star, path, cycle and complete graph, respectively.

For a connected graph G, the radius $r(G)$ and the diameter $D(G)$ are, respectively, the minimum and the maximum eccentricities of the vertices of G. The set of all vertices of minimum eccentricity is the center of a graph. A tree has exactly one central vertex or two adjacent central vertices. For a tree T, if T has one central vertex, then $D(T) = 2r(D)$; if T has two adjacent central vertices, then $D(T) = 2r(T) - 1$.

For a subset M of $V(G)$ ($E(G)$, respectively), $G - M$ denotes the graph obtained from G by deleting the vertices in M and their incident edges (the edges in M, respectively). For a subset M of the edge set of the complement of G, $G + M$ denotes the graph obtained from G by adding the edges in M. In the case M is a single vertex $\{v\}$ (edge $\{e\}$, respectively), then $G - M$ is denoted by $G - v$ ($G - e$, respectively), and $G + \{e\}$ is denoted by $G + e$.

2 Zagreb eccentricity indices and domination number

A subset S of $V(G)$ is called a domination set of the graph G if for every vertex $u \in V(G) \setminus S$, there exists a vertex $v \in S$ such that u is adjacent to v. The domination number of G, denoted by $\gamma(G)$, is defined as the minimum cardinality of domination sets of G. For an n-vertex connected graph G, it is known [14] that $\gamma(G) \leq \lfloor \frac{n}{2} \rfloor$. The equality case was characterized independently in [5, 22]. Let $\mathbb{T}_{n,\gamma}$ be the set of n-vertex trees with domination number γ, where $1 \leq \gamma \leq \lfloor \frac{n}{2} \rfloor$. Note that $\mathbb{T}_{n,1} = \{S_n\}$. Therefore, we can suppose that $2 \leq \gamma \leq \lfloor \frac{n}{2} \rfloor$.

A matching M of the graph G is a subset of $E(G)$ such that no two edges in M share a common vertex. The matching number of G, denoted by $\beta(G)$, is defined as the maximum cardinality of matchings of G. For an n-vertex graph, if $n = 2\beta(G)$, then G has a perfect matching. Obviously, S_n is the unique n-vertex graph with the matching number $\beta = 1$.

It has been shown in [1] that a graph G without isolated vertices has a $\gamma(G)$-set S such that for each vertex $u \in S$, there exists a vertex in $V(G) \setminus S$ that is adjacent to u but no other vertices in S. Thus we have the following lemma.

Lemma 2.1 *For a graph G, we have $\gamma(G) \leq \beta(G)$.*

For $3 \leq \beta \leq \lfloor \frac{n}{2} \rfloor$, let $T_{n,\beta}$ be the tree obtained by attaching $\beta - 1$ paths on two vertices to the central vertex of the star $S_{n-2\beta+2}$. Obviously, the matching number of $T_{n,\beta}$ is β.

Lemma 2.2 [21] *Let T be an n-vertex tree with matching number β.*

(*i*) *If $\beta(T) = 2$, then $\xi_1(T) \geq 9n - 10$ and $\xi_2(T) \geq 6n - 8$ with either equality if and only if T has diameter 3.*

(*ii*) *If $3 \leq \beta(T) \leq \lfloor \frac{n}{2} \rfloor$, then $\xi_1(T) \geq 9n + 7\beta - 12$ and $\xi_2(T) \geq 6n + 6\beta - 12$ with either equality if and only if $T \cong T_{n,\beta}$.*

Lemma 2.3 *Let T be an n-vertex tree with $n \geq 4$, and $e = uv$ be a non-pendent edge of T. Let T' be the tree obtained from T by deleting e, identifying u and v, denoted by u', and attaching a vertex v' to u'. Then we have $\xi_1(T') < \xi_1(T)$ and $\xi_2(T') < \xi_2(T)$.*

Proof. Let $T - e = T_1 \cup T_2$ with $u \in V(T_1)$ and $v \in V(T_2)$. Let x be a pendent vertex with $e_{T_1}(u) = d_{T_1}(u, x)$ and y a pendent vertex with $e_{T_2}(v) = d_{T_2}(v, y)$. Suppose without loss of generality that $d_{T_1}(u, x) \geq d_{T_2}(v, y)$. Obviously, $d_{T_1}(u, x) = d_{T'}(u', x)$ and $d_{T_2}(v, y) = d_{T'}(u', y)$. Note that $e_{T'}(w) \leq e_T(w)$ for any $w \in V(T) \setminus \{v, y\}$,

$$e_T(v) = 1 + d_{T_1}(u, x) = 1 + d_{T'}(u', x) = e_{T'}(v')$$

and

$$e_T(y) = d_{T_2}(y, v) + 1 + d_{T_1}(u, x) > d_{T'}(y, u') + d_{T'}(u', x) = e_{T'}(y).$$

Let z be the neighbor of y. Then

$$\begin{aligned} & \xi_1(T') - \xi_1(T) \\ = & \sum_{w \in V(T) \setminus \{v,y\}} [e^2_{T'}(w) - e^2_T(w)] + e^2_{T'}(v') - e^2_T(v) + e^2_{T'}(y) - e^2_T(y) \\ \leq & \ e^2_{T'}(y) - e^2_T(y) < 0, \end{aligned}$$

and $\xi_2(T') - \xi_2(T) \leq e_{T'}(y) e_{T'}(z) - e_T(y) e_T(z) < 0$. ■

Lemma 2.4 *If $T^* \in \mathbb{T}_{n,\gamma}$ has the minimum Zagreb eccentricity index ξ_1 (ξ_2, respectively), then $\gamma(T^*) = \beta(T^*) = \gamma$.*

Proof. Suppose that $\gamma = \gamma(T^*) < \beta(T^*)$. Let $S = \{w_1, w_2, \cdots, w_\gamma\}$ be a dominating set of T^*. Then there exist γ edges $w_1w'_1, w_2w'_2, \cdots, w_\gamma w'_\gamma$ in T^*, where $w'_i \in V(T^*) \setminus S$ for $i = 1, 2, \cdots, \gamma$. Since $\gamma = \gamma(T^*) < \beta(T^*)$, there must exist another edge, say v_1v_2, which is independent of each edge $w_iw'_i$ for $i = 1, 2, \cdots, \gamma$.

Since T^* is a tree, v_1 and v_2 cannot be dominated by the same vertex in S, and thus v_1 and v_2 are dominated by two different vertices in S, say v_i is dominated by w_i for $i = 1, 2$. Note that $deg(v_1)$, $deg(v_2) \geq 2$ and $deg(w_1)$, $deg(w_2) \geq 2$. Then we can obtain an n-vertex tree $T^{*\prime}$ by applying the transformation in Lemma 2.3 on the edge v_1w_1 or v_2w_2, and $\xi_1(T^{*\prime}) < \xi_1(T^*)$ and $\xi_2(T^{*\prime}) < \xi_2(T^*)$, a contradiction. Thus $\gamma(T^*) \geq \beta(T^*)$. Now the result follows from Lemma 2.1. ■

Combining Lemmas 2.2 and 2.4, the following proposition is obvious.

Proposition 2.1 *Let $T \in \mathbb{T}_{n,\gamma}$, where $2 \leq \gamma \leq \lfloor \frac{n}{2} \rfloor$.*

(i) If $\gamma = 2$, then $\xi_1(T) \geq 9n - 10$ and $\xi_2(T) \geq 6n - 8$ with either equality if and only if T has diameter 3.

(ii) If $3 \leq \gamma \leq \lfloor \frac{n}{2} \rfloor$, then $\xi_1(T) \geq 9n + 7\gamma - 12$ and $\xi_2(T) \geq 6n + 6\gamma - 12$ with either equality if and only if $T \cong T_{n,\gamma}$.

The corona of two graphs G_1 and G_2 is a graph $G = G_1 \circ G_2$ obtained from one copy of G_1 with $|V(G_1)|$ copies G_2, where the i-th vertex of G_1 is adjacent to every vertex in the i-th copy of G_2. In particular, for a positive integer k, we denote by $G^{(k)}$ the graph $G \circ kK_1$, where kK_1 is the graph consisting of k isolated vertices.

Lemma 2.5 [5, 22] *If $n = 2\gamma$, then a tree T belongs to $\mathbb{T}_{n,\gamma}$ if and only if there exists a γ-vertex tree H such that $T = H \circ K_1$.*

The eccentric connectivity index and the average eccentricity of G are defined as

$$\xi^c(G) = \sum_{u \in V(G)} deg(u) \cdot e(u)$$

and

$$avec(G) = \frac{1}{|V(G)|} \sum_{u \in V(G)} e(u),$$

respectively [15, 16].

Lemma 2.6 [17, 21, 25] *Let T be an n-vertex tree. Then $\xi_1(S_n) \leq \xi_1(T) \leq \xi_1(P_n)$, $\xi_2(S_n) \leq \xi_2(T) \leq \xi_2(P_n)$, $\xi^c(S_n) \leq \xi^c(T) \leq \xi^c(P_n)$ and $avec(S_n) \leq avec(T) \leq avec(P_n)$, with any left equality if and only if $T \cong S_n$ and any right equality if and only if $T \cong P_n$.*

Lemma 2.7 *Let T be an n-vertex tree and $T^{(k)} = T \circ kK_1$. Then $\xi_1(S_n^{(k)}) \leq \xi_1(T^{(k)}) \leq \xi_1(P_n^{(k)})$ and $\xi_2(S_n^{(k)}) \leq \xi_2(T^{(k)}) \leq \xi_2(P_n^{(k)})$, with either left equality if and only if $T \cong S_n$ and either right equality if and only if $T \cong P_n$.*

Proof. Let uv be a pendent edge of $T^{(k)}$ with $deg_{T^{(k)}}(v) = 1$, then $e_{T^{(k)}}(v) = e_{T^{(k)}}(u)+1$. Moreover, $e_{T^{(k)}}(x) = e_T(x)+1$ for any $x \in V(T)$. By the definitions of Zagreb eccentricity indices ξ_1 and ξ_2, we have

$$\begin{aligned}
\xi_1(T^{(k)}) &= \sum_{x\in V(T^{(k)})} e^2_{T^{(k)}}(x) = \sum_{x\in V(T)} e^2_{T^{(k)}}(x) + k \sum_{x\in V(T)} [e_{T^{(k)}}(x)+1]^2 \\
&= \sum_{x\in V(T)} [e_T(x)+1]^2 + k \sum_{x\in V(T)} [e_T(x)+2]^2 \\
&= \sum_{x\in V(T)} [e^2_T(x)+2e_T(x)+1] + k \sum_{x\in V(T)} [e^2_T(x)+4e_T(x)+4] \\
&= (1+k) \sum_{x\in V(T)} e^2_T(x) + (2+4k) \sum_{x\in V(T)} e_T(x) + n + 4nk \\
&= (1+k)\xi_1(T) + n(2+4k)avec(T) + n + 4nk,
\end{aligned}$$

$$\begin{aligned}
\xi_2(T^{(k)}) &= \sum_{xy\in E(T^{(k)})} e_{T^{(k)}}(x)e_{T^{(k)}}(y) \\
&= \sum_{xy\in E(T)} e_{T^{(k)}}(x)e_{T^{(k)}}(y) + k \sum_{x\in V(T)} e_{T^{(k)}}(x)[e_{T^{(k)}}(x)+1] \\
&= \sum_{xy\in E(T)} [e_T(x)+1][e_T(y)+1] + k \sum_{x\in V(T)} [e_T(x)+1][e_T(x)+2] \\
&= \sum_{xy\in E(T)} e_T(x)e_T(y) + \sum_{xy\in E(T)} [e_T(x)+e_T(y)] + n - 1 \\
&\quad + k \sum_{x\in V(T)} e^2_T(x) + 3k \sum_{x\in V(T)} e_T(x) + 2nk \\
&= \xi_2(T) + \xi^c(T) + k\xi_1(T) + 3nk \cdot avec(T) + n - 1 + 2nk.
\end{aligned}$$

By Lemma 2.6, the result follows easily. ■

Proposition 2.2 *Let $T \in \mathbb{T}_{n,\gamma}$. If $\gamma = \frac{n}{2}$, then*

$$\xi_1(S_{\frac{n}{2}} \circ K_1) \leq \xi_1(T) \leq \xi_1(P_{\frac{n}{2}} \circ K_1)$$

and

$$\xi_2(S_{\frac{n}{2}} \circ K_1) \leq \xi_2(T) \leq \xi_2(P_{\frac{n}{2}} \circ K_1)$$

with any left equality if and only if $T \cong S_{\frac{n}{2}} \circ K_1$, i.e., Proposition 2.1 for $\gamma = \frac{n}{2}$, and any right equality if and only if $T \cong P_{\frac{n}{2}} \circ K_1$.

Proof. By Lemma 2.5, we have any tree in $\mathbb{T}_{n,\frac{n}{2}}$ must be of the form $H \circ K_1$, where H is a $\frac{n}{2}$-vertex tree. Taking $k = 1$ in Lemma 2.7 proves the result. ■

Proposition 2.3 *Let $T \in \mathbb{T}_{n,\gamma}$. If $\gamma = \lceil \frac{n}{3} \rceil$, then $\xi_1(T) \leq \xi_1(P_n)$ and $\xi_2(T) \leq \xi_2(P_n)$ with either equality if and only if $T \cong P_n$.*

Proof. Note that $\gamma(P_n) = \lceil \frac{n}{3} \rceil$. By Lemma 2.6, the result follows. ■

Let $P_{n,s}(a,b)$ be an n-vertex tree obtained by attaching a and b pendent vertices to the two terminal vertices of P_s with $s \geq 2$, respectively, where $a, b \geq 0$ and $a + b = n - s$. Let $\mathbb{P}_{n,s} = \{P_{n,s}(a,b) : a, b \geq 0, a + b = n - s\}$.

Proposition 2.4 *Let $T \in \mathbb{T}_{n,\gamma}$.*

- *(i) If $\gamma = 2$ and $n = 4, 5, 6$, then $\xi_1(T) \leq \xi_1(P_n)$ and $\xi_2(T) \leq \xi_2(P_n)$ with either equality if and only if $T \cong P_n$.*
- *(ii) If $\gamma = 2$ and $n \geq 7$, then $\xi_1(T) \leq 25n - 50$ and $\xi_2(T) \leq 20n - 47$ with either equality if and only if $T \in \mathbb{P}_{n,4}$.*

Proof. By Proposition 2.3, the cases $n = 4, 5, 6$ are obvious. Suppose that $n \geq 7$. Let T^* be a tree in $\mathbb{T}_{n,2}$ with maximum Zagreb eccentricity index ξ_1(ξ_2, respectively), and $S^* = \{w_1, w_2\}$ be a dominating set of T^*. Let a and b be the numbers of pendent neighbors of w_1 and w_2 in T^*, respectively, where $a \geq b \geq 0$.

Suppose that $w_1w_2 \in E(T^*)$. Then $T^* \in \mathbb{P}_{n,2}$. Since $a + b = n - 2 \geq 5$ and $\gamma = 2$, we have $a \geq b \geq 1$. Let x be a pendent neighbor of w_1, and $T_1^* = T^* - w_1w_2 + xw_2$. Then $T_1^* \in \mathbb{T}_{n,2}$. By Lemma 2.3, $\xi_1(T^*) < \xi_1(T_1^*)$ and $\xi_2(T^*) < \xi_2(T_1^*)$, a contradiction. Thus $w_1w_2 \notin E(T)$, i.e., $d_{T^*}(w_1, w_2) \geq 2$.

If $d_{T^*}(w_1, w_2) \geq 4$, then there exists at least one vertex y on the shortest path between w_1 and w_2 such that y can not be dominated by the two vertices w_1 and w_2, a contradiction. Thus $2 \leq d_{T^*}(w_1, w_2) \leq 3$. Suppose that $d_{T^*}(w_1, w_2) = 2$. Then $T^* \in \mathbb{P}_{n,3}$. Since $a + b = n - 3 \geq 4$ and $\gamma = 2$, we have $a > 0$. Let z be a pendent neighbor of w_1 in T^* and w be the common neighbor of w_1 and w_2. Let $T_2^* = T^* - w_1w + zw$. Then $T_2^* \in \mathbb{T}_{n,2}$. By Lemma 2.3, we have $\xi_1(T^*) < \xi_1(T_2^*)$ and $\xi_2(T^*) < \xi_2(T_2^*)$, a contradiction. Thus $d_{T^*}(w_1, w_2) = 3$.

It follows that $T^* \in \mathbb{P}_{n,4}$, and then $\xi_1(T^*) = 25n - 50$ and $\xi_2(T^*) = 20n - 47$. ■

3 Zagreb eccentricity indices and maximum degree

Denote by $\Delta = \Delta(T)$ the maximum vertex degree of a tree T. Let $\mathbb{T}(n, \Delta)$ be the set of all n-vertex trees with maximum degree Δ, where $2 \leq \Delta \leq n-1$. Note that $\mathbb{T}(n, 2) = \{P_n\}$ and $\mathbb{T}(n, n-1) = \{S_n\}$. Therefore, we can suppose that $3 \leq \Delta \leq n-2$.

Lemma 3.1 *Let T be a rooted tree with a central vertex c as root, and w be a pendent vertex most distant from the root, adjacent to vertex v. Let u $(u \neq v)$ be the vertex closest to the root vertex, such that $deg(u) < \Delta$ and $e(u) \leq e(v)$. Consider $T' = T - vw + uw$. Then $\xi_1(T') \leq \xi_1(T)$ and $\xi_2(T') \leq \xi_2(T)$ with either equality if and only if $e(u) = e(v)$ and $D(T') = D(T)$.*

Proof. Since T is rooted at the central vertex c, we have $d(c, w) = r(T)$ and $d(c, v) = r(T) - 1$. Furthermore, there exists a pendent vertex w' in a different subtree attached to the central vertex c, such that $d(c, w') = r(T)$ or $d(c, w') = r(T) - 1$. Then $e(w') = 2r(T) > 2r(T) - 1 = e(v)$ for T with one central vertex, while $e(w') = 2r(T) - 1 > 2r(T) - 2 = e(v)$ for T with two adjacent central vertices. Combined with $e(v) \geq e(u)$, we have $d(c, w') > d(c, u)$, i.e., $w' \neq u$.

Note that $e_{T'}(x) \leq e_T(x)$ for any $x \in V(T)$. Furthermore, rotating the edge vw to uw, all the eccentricities of vertices other than w remain the same if and only if $D(T') = D(T)$.

If $D(T') < D(T)$, then

$$\begin{aligned}\xi_1(T') - \xi_1(T) &< e^2_{T'}(w) - e^2_T(w) = [e_{T'}(u) + 1]^2 - [e_T(v) + 1]^2 \\ &< [e_T(u) + 1]^2 - [e_T(v) + 1]^2 \leq 0,\end{aligned}$$

$$\begin{aligned}\xi_2(T') - \xi_2(T) &< e_{T'}(u)e_{T'}(w) - e_T(v)e_T(w) \\ &< e_T(u)[e_T(u) + 1] - e_T(v)[e_T(v) + 1] \leq 0,\end{aligned}$$

and thus $\xi_1(T') < \xi_1(T)$ and $\xi_2(T') < \xi_2(T)$.

If $D(T') = D(T)$, then

$$\begin{aligned}\xi_1(T') - \xi_1(T) &= e^2_{T'}(w) - e^2_T(w) = [e_{T'}(u) + 1]^2 - [e_T(v) + 1]^2 \\ &= [e_T(u) + 1]^2 - [e_T(v) + 1]^2 \leq 0,\end{aligned}$$

$$\xi_2(T') - \xi_2(T) = e_{T'}(u)e_{T'}(w) - e_T(v)e_T(w)$$

$$= \quad e_T(u)[e_T(u)+1] - e_T(v)[e_T(v)+1] \leq 0,$$

and thus $\xi_1(T') \leq \xi_1(T)$ and $\xi_2(T') \leq \xi_2(T)$ with either equality if and only if $e(u) = e(v)$.
■

For a rooted tree T with a central vertex c as root, the i-th level in T is a subset of $V(T)$ such that the distance from c to any vertex in the i-th level is i, where $0 \leq i \leq r(T)$.

The Volkmann tree $\mathcal{VT}(n,\Delta)$ is an n-vertex tree with maximum degree Δ defined as follows [6,7]. Start with the root having Δ children. Every vertex different from the root, which is not on one of the last two levels, has exactly $\Delta - 1$ children. On the last level, while not all vertices need to exist, the vertices that do exist fill the level consecutively. Thus, at most one vertex on the second last level has its degree different from 1 and Δ. Let $\mathbb{VT}(1)$ be the set of n-vertex trees with maximum degree Δ, obtained from the Volkmann tree $\mathcal{VT}(n,\Delta)$ by arranging the vertices on the last level arbitrarily in at least two subtrees attached to the root vertex. Let $\mathbb{VT}(2)$ be the set of n-vertex trees with maximum degree Δ, obtained from the Volkmann tree $\mathcal{VT}(n,\Delta)$, in which not all vertices on the last two levels need to exist, the vertices that do exist on the last two levels are arranged arbitrarily, but all the vertices on the last level are in one subtree attached to the root vertex and the second last level in this subtree is full. For example, $T_1 \in \mathbb{VT}(1)$ with $n = 28$ and $\Delta = 4$, and $T_2 \in \mathbb{VT}(2)$ with $n = 22$ and $\Delta = 4$ are shown in Figure 1.

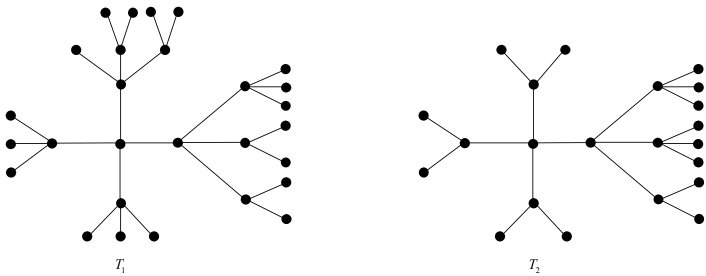

Figure 1: The trees T_1 and T_2 in $\mathbb{VT}(1)$ and $\mathbb{VT}(2)$, respectively.

For a tree $T \in \mathbb{T}(n,\Delta)$, let $k = k(n,\Delta)$ be the greatest integer such that

$$n \geq 1 + \Delta + \Delta(\Delta-1) + \Delta(\Delta-1)^2 + \cdots + \Delta(\Delta-1)^{k-1},$$

and let

$$N = 1 + \Delta + \Delta(\Delta-1) + \Delta(\Delta-1)^2 + \cdots + \Delta(\Delta-1)^{k-1}.$$

Proposition 3.1 *Among the trees in* $\mathbb{T}(n,\Delta)$,

(*i*) *for* $n = N$, $\mathcal{VT}(n,\Delta)$ *is the unique tree with minimum indices* ξ_1 *and* ξ_2;

(*ii*) *for* $N < n \leq N + (\Delta-1)^k$, *the trees in* $\mathbb{VT}(2)$ *are the unique trees with minimum indices* ξ_1 *and* ξ_2;

(*iii*) *for* $N + (\Delta-1)^k < n < N + \Delta(\Delta-1)^k$, *the trees in* $\mathbb{VT}(1)$ *are the unique trees with minimum indices* ξ_1 *and* ξ_2.

Proof. Let T^* be the extremal tree in $\mathbb{T}(n,\Delta)$ with minimum Zagreb eccentricity index ξ_1 (ξ_2, respectively). Suppose that T^* is a rooted tree with a central vertex c as root. Let w be the pendent vertex most distant from the root, adjacent to vertex v. Then we have a fact that

$$e(v) = \begin{cases} 2r(T^*) - 1 & \text{if } T^* \text{ has one central vertex} \\ 2r(T^*) - 2 & \text{if } T^* \text{ has two adjacent central vertices.} \end{cases}$$

Let u be a vertex closest to the root vertex c such that $deg(u) < \Delta$. Then we have another fact that if T^* has two adjacent central vertices, and u and v lie on the same subtree attached to the vertex c, then $e(u) = d(c,u) + r(T^*) - 1$; otherwise, $e(u) = d(c,u) + r(T^*)$.

Let $k = k(n,\Delta)$. It can be easily seen that $r(T^*) \geq k$ by the definition of k. Suppose that $r(T^*) = d(c,w) > k+1$, i.e., $r(T^*) \geq k+2$. By the definitions of u and k, we have $d(c,u) \leq k$, and then $e(u) \leq d(c,u) + r(T^*) \leq k + r(T^*)$, which implies that $e(v) \geq 2r(T^*) - 2 \geq r(T^*) + k \geq e(u)$.

Suppose that $e(v) > e(u)$. Let $T^{*\prime} = T - vw + uw$. By Lemma 3.1, $\xi_1(T^{*\prime}) < \xi_1(T^*)$ and $\xi_2(T^{*\prime}) < \xi_2(T^*)$, a contradiction. Thus $e(v) = e(u)$. Then $e(u) = d(c,u) + r(T^*)$ and $e(v) = 2r(T^*) - 2$, which, together with the above two facts, implies that T^* has two adjacent central vertices, and u and v lie on different subtrees attached to the vertex c. Furthermore, $d(c,u) = k$ and $r(T^*) = k+2$, which implies that u, v and w belong to the k-th, $(k+1)$-th and $(k+2)$-th levels, respectively. If there exists at least one diametrical path in T^* not containing edge vw, then applying the transformation in Lemma 3.1 on these diametrical paths do not change $D(T^*)$. According to the definition of k, after finite times of the transformation, vertex w will be the only vertex at distance $r(T^*)$ from the vertex c, and applying the transformation in Lemma 3.1 on vw will strictly decrease $D(T^*)$, resulting smaller ξ_1 and ξ_2, also a contradiction. Thus $k \leq r(T^*) \leq k+1$.

If $r(T^*) = k$, then $n = N$, and the Volkmann tree $\mathcal{VT}(n, \Delta)$ is the unique tree with the minimum ξ_1 and ξ_2, proving (i).

Now suppose that $r(T^*) = k + 1$. If $d(c, u) < k - 1$, then $e(v) \geq 2r(T^*) - 2 = r(T^*) + k - 1 > r(T^*) + d(c, u) \geq e(u)$, i.e., $e(v) > e(u)$. Applying the transformation in Lemma 3.1 can strictly decrease ξ_1 and ξ_2, a contradiction. Thus $k - 1 \leq d(c, u) \leq k$, i.e., the 1-th, 2-th, $\cdots$, $(k-1)$-th levels are full (the i-th level contains exactly $\Delta(\Delta-1)^{i-1}$ vertices for each $i = 1, 2, \cdots, k-1$), while the k-th and $(k+1)$-th levels contain $M = n - [1 + \Delta + \Delta(\Delta-1) + \Delta(\Delta-1)^2 + \cdots + \Delta(\Delta-1)^{k-2}]$ vertices.

Next we prove (iii). Suppose that $M > \Delta(\Delta-1)^{k-1} + (\Delta-1)^k$, where $(\Delta-1)^k$ is the maximum number of vertices on the $(k+1)$-th level in one subtree attached to the vertex c. Then T^* has only one central vertex, i.e., $D(T^*) = 2r(T^*)$ and $e(v) = 2r(T^*) - 1 = 2k + 1$. If $d(c, u) = k - 1$, then $e(u) = d(c, u) + r(T^*) = k - 1 + k + 1 = 2k < e(v)$. Then applying the transformation in Lemma 3.1 can strictly decrease ξ_1 and ξ_2, a contradiction. Thus $d(c, u) = k$, i.e., the k-th level is also full and the pendent vertices in $(k+1)$-th level can be arbitrary assigned in at least two subtrees attached to the vertex c, i.e., $T^* \in \mathbb{VT}(1)$, proving (iii).

Now we prove (ii). For $\Delta(\Delta-1)^{k-1} < M \leq \Delta(\Delta-1)^{k-1} + (\Delta-1)^k$, if T^* has only one central vertex, by the same argument as above, we have $d(c, u) = k$, i.e., the k-th level is also full and the $(k+1)$-th level has at most $(\Delta-1)^k$ pendent vertices in at least two subtrees attached to the vertex c. After finite times of the transformation in Lemma 3.1 with unchanged ξ_1 and ξ_2, the vertex w will be the only vertex at distance $r(T^*)$ from the vertex c in one subtree attached to the vertex c, and other vertices on the $(k+1)$-th level are all in another subtree attached to the vertex c. Then applying the transformation in Lemma 3.1 on vw will strictly decrease $D(T^*)$, resulting smaller ξ_1 and ξ_2, also a contradiction. Thus T^* must have two adjacent central vertices, i.e., $D(T^*) = 2r(T^*) - 1$ and $e(v) = 2r(T^*) - 2 = 2k$. If $d(c, u) = k-1$, and u and v are in the same subtree attached to the vertex c, then $e(u) = d(c, u) + r(T^*) - 1 = k - 1 + k + 1 - 1 = 2k - 1 < e(v)$, and applying the transformation in Lemma 3.1 can strictly decrease ξ_1 and ξ_2, a contradiction. If $d(c, u) = k - 1$, and u and v are not in the same subtree attached to the vertex c, then $e(u) = d(c, u) + r(T^*) = k - 1 + k + 1 = 2k = e(v)$, which, together with Lemma 3.1 and the definition of k, implies that applying the transformation in Lemma 3.1 to fill the k-th level do not change $D(T^*)$, resulting unchanged ξ_1 and ξ_2. Then $T^* \in \mathbb{VT}(2)$. If

$d(c,u)=k$, then the k-th level is also full and the pendent vertices on the $(k+1)$-th level are in the same subtree attached to the vertex c, i.e., $T^* \in \mathbb{VT}(2)$. The (ii) follows. ■

4 Zagreb eccentricity indices and bipartition size

Let G be an n-vertex connected bipartite graph. Hence its vertex set can be uniquely partitioned into two subsets V_1 and V_2 such that each edge joins a vertex in V_1 with a vertex in V_2. If V_1 has p vertices and V_2 has q vertices, where $p \le q$ and $p+q=n$, then we say that (p,q) is the bipartition size of G. Let $\mathbb{T}_n^{p,q}$ be the set of n-vertex trees with bipartition size (p,q). Obviously, $\mathbb{T}_n^{1,n-1}=\{S_n\}$.

Lemma 4.1 *Let $P=\cdots uvww_1$ be a diametrical path of a tree T, where w has t $(t\ge 1)$ pendent neighbors $w_1,w_2,\cdots,w_t$ in T. Denote by T_v the component of $T-\{u,w\}$ which contains vertex v. Consider $T'=T-\{ww_1,ww_2,\cdots,ww_t\}+\{uw_1,uw_2,\cdots,uw_t\}$.*

(i) If $D(T)=4$ and $e_{T_v}(v)=2$, then $\xi_1(T')=\xi_1(T)$ and $\xi_2(T')=\xi_2(T)$.

(ii) If $D(T)=4$ and $e_{T_v}(v)=0,1$, or $D(T)\ge 5$ then $\xi_1(T')<\xi_1(T)$ and $\xi_2(T')<\xi_2(T)$.

Proof. If $D(T)=4$ and $e_{T_v}(v)=2$, it can be easily seen that $e_{T'}(x)=e_T(x)$ for any $x\in V(T)$, proving (i).

Now we prove (ii). Let $T_0=T-\{w_1,w_2,\cdots,w_t\}$. It can be easily seen that $e_{T'}(x)\le e_T(x)$ for any $x\in V(T_0)$, $e_T(w_i)=e_T(w)+1$ and $e_{T'}(w_i)=e_{T'}(u)+1$ for $i=1,2,\cdots,t$. If $D(T)=4$ and $e_{T_v}(v)=0,1$, then $e_T(w)=3$, $e_{T'}(u)=2$, and thus

$$\begin{aligned}
\xi_1(T')-\xi_1(T) &= \sum_{x\in V(T_0)}\left[e_{T'}^2(x)-e_T^2(x)\right]+t\cdot e_{T'}^2(w_1)-t\cdot e_T^2(w_1)\\
&\le t\left[e_{T'}(u)+1\right]^2-t\left[e_T(w)+1\right]^2\\
&= 9t-16t=-7t<0,
\end{aligned}$$

$$\begin{aligned}
\xi_2(T')-\xi_2(T) &= \sum_{xy\in E(T_0)}\left[e_{T'}(x)e_{T'}(y)-e_T(x)e_T(y)\right]\\
&\quad +t\cdot e_{T'}(u)e_{T'}(w_1)-t\cdot e_T(w)e_T(w_1)\\
&\le t\cdot e_{T'}(u)[e_{T'}(u)+1]-t\cdot e_T(w)[e_T(w)+1]\\
&= 6t-12t=-6t<0,
\end{aligned}$$

implying that $\xi_1(T') < \xi_1(T)$ and $\xi_2(T') < \xi_2(T)$. If $D(T) \geq 5$, then $e_T(u) \leq e_T(v) < e_T(w)$, and thus

$$\begin{aligned}
\xi_1(T') - \xi_1(T) &= \sum_{x \in V(T_0)} \left[e^2_{T'}(x) - e^2_T(x)\right] + t \cdot e^2_{T'}(w_1) - t \cdot e^2_T(w_1) \\
&\leq t\left[e_{T'}(u) + 1\right]^2 - t\left[e_T(w) + 1\right]^2 \\
&\leq t\left[e_T(u) + 1\right]^2 - t\left[e_T(w) + 1\right]^2 < 0,
\end{aligned}$$

$$\begin{aligned}
\xi_2(T') - \xi_2(T) &= \sum_{xy \in E(T_0)} \left[e_{T'}(x)e_{T'}(y) - e_T(x)e_T(y)\right] \\
&\quad + t \cdot e_{T'}(u)e_{T'}(w_1) - t \cdot e_T(w)e_T(w_1) \\
&\leq t \cdot e_{T'}(u)[e_{T'}(u) + 1] - t \cdot e_T(w)[e_T(w) + 1] \\
&\leq t \cdot e_T(u)[e_T(u) + 1] - t \cdot e_T(w)[e_T(w) + 1] < 0,
\end{aligned}$$

implying that $\xi_1(T') < \xi_1(T)$ and $\xi_2(T') < \xi_2(T)$. ■

Let $T_n^{p,q}$ be the n-vertex tree obtained by attaching $p-1$ and $q-1$ pendent vertices $u_1, u_2, \cdots, u_{p-1}$ and $v_1, v_2, \cdots, v_{q-1}$ to the two vertices u, v on P_2, respectively, where $2 \leq p \leq q$ and $p + q = n$.

Proposition 4.1 *Let $\mathbb{T}_n^{p,q}$ with $n \geq 4$ and $2 \leq p \leq \lfloor \frac{n}{2} \rfloor$. Then $T_n^{p,q}$ is the unique graph with minimum indices ξ_1 and ξ_2, which are equal to $9n - 10$ and $6n - 8$, respectively.*

Proof. Let $T \in \mathbb{T}_n^{p,q}$. Then $D(T) \geq 3$. If $D(T) = 3$, then $T = T_n^{p,q}$. Suppose that $D(T) \geq 4$. If $D(T) \geq 5$, then we can repeat to apply the transformation in Lemma 4.1 (ii) on diametrical paths in T to obtain a tree in $\mathbb{T}_n^{p,q}$ of diameter 4 with smaller ξ_1 and ξ_2. If $D(T) = 4$ and the central vertex of T has more than two non-pendent neighbors, then we can repeat to apply the transformation in Lemma 4.1 (i) on diametrical paths in T to obtain a tree in $\mathbb{T}_n^{p,q}$ whose central vertex has exactly two non-pendent neighbors with unchanged ξ_1 and ξ_2. If $D(T) = 4$ and the central vertex of T has exactly two non-pendent neighbors, then we can apply the transformation in Lemma 4.1 (ii) on a diametrical path in T to obtain the tree $T_n^{p,q}$ of diameter 3 with smaller ξ_1 and ξ_2. By direct calculation, we have $\xi_1(T_n^{p,q}) = 9n - 10$ and $\xi_2(T_n^{p,q}) = 6n - 8$. ■

Let $\mathcal{T}_s^p$ be the set of n-vertex tree obtained from $T_n^{p,q}$ by deleting s $(1 \leq s \leq p-2)$ pendent vertices $u_1, u_2, \cdots, u_s$ and attaching them to some of $v_1, v_2, \cdots, v_{q-1}$. Let $\mathbf{T}_t^q$ be the set of n-vertex tree obtained from $T_n^{p,q}$ by deleting t $(1 \le t \le q-2)$ pendent vertices $v_1, v_2, \cdots, v_t$ and attaching them to some of $u_1, u_2, \cdots, u_{p-1}$. Let $\mathbb{T}^p = \cup_{1 \le s \le p-2} \mathcal{T}_s^p$ and $\mathbf{T}^q = \cup_{1 \le t \le q-2} \mathbf{T}_t^q$.

Proposition 4.2 *Among the graphs in $\mathbb{T}_n^{p,q}$ with $n \ge 5$ and $2 \le p \le \lfloor \frac{n}{2} \rfloor$,*

(i) if $p \ge 3$, then the graphs in $\mathbb{T}^p$ are the unique graphs with second-minimum indices ξ_1 and ξ_2, which are equal to $16p + 9q - 12$ and $12p + 6q - 12$, respectively;

(ii) if $p = 2$, then the graphs in $\mathbf{T}^q$ are the unique graphs with second-minimum indices ξ_1 and ξ_2, which are equal to $16q + 6$ and $12q$, respectively.

Proof. By the proof of Proposition 4.1, the diameter of the graphs in $\mathbb{T}_n^{p,q}$ with the second-minimum indices ξ_1 and ξ_2 must be 4. Thus such graphs belong to $\mathbb{T}^p$ or $\mathbf{T}^q$ if $p \ge 3$, and belong to $\mathbf{T}^q$ if $p = 2$. For any $T_1 \in \mathbb{T}^p$ and $T_2 \in \mathbf{T}^q$ with $p \ge 3$, by direct calculation, we have

$$\xi_1(T_1) = 16p + 9q - 12 \le 16q + 9p - 12 = \xi_1(T_2)$$

and

$$\xi_2(T_1) = 12p + 6q - 12 \le 12q + 6p - 12 = \xi_2(T_2)$$

with either equality if and only if $p = q$. ■

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