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On Segments, Vertices of Degree Two and the First Zagreb Index of Trees

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Abstract

The first Zagreb index M_1 of a graph G is equal to the sum of squares of the vertex degrees of G. A segment of a tree is a path-subtree whose terminal vertices are branching or pendent vertices. In this paper, we characterize the trees which minimize and maximize the first Zagreb index among all trees with fixed number of segments, respectively. As a byproduct, we also prove that these trees also share the minimum and maximum first Zagreb index among all trees with fixed number of vertices of degree two, respectively.

1 Introduction

In this paper, we only consider the connected and simple graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex v in G is the number of edges of G incident with v. The maximum vertex degree of G is denote by $\triangle(G)$. The first Zagreb index M_1 and the second Zagreb index M_2 of G are defined as

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

The Zagreb indices M_1 and M_2 were introduced in [6] and elaborated in [7]. They reflect the extent of branching of the underlying molecular structure. Chemists are often interested in the Zagreb indices of certain trees which represent some acyclic molecular structures. The main properties of M_1 and M_2 of trees were summarized in [1, 5]. The extremal trees that maximize or minimize Zagreb indices within certain classes of trees received great attention, see [10] for trees with fixed maximum degree, [3, 4, 8] for trees with given number of pendent vertices, [9] for trees with given degree sequences, [11] for trees with perfect matchings and [12] for the chemical trees (trees with maximum degrees at most 4).

A vertex of degree one of a tree is called a *pendent vertex*. A vertex of a tree T with degree 3 or greater is called a *branching vertex* of T. In the sequel, we always use the symbols $V_1(T)$, $V_2(T)$ and $V_{\geq 3}(T)$ to denote the set of pendent vertices, the set of vertices of degree two and the set of branching vertices in a tree T, respectively. Thus the vertex set of any tree T can be partitioned into

$$V(T) = V_1(T) \cup V_2(T) \cup V_{\geq 3}(T).$$

Recently, Goubko and Gutman [3, 4] characterized the trees with the minimum first Zagreb index among all trees with fixed number of pendent vertices. So, it is natural to consider the analogous problem for the trees with fixed number of vertices of degree two.

Problem A. Characterize the trees which maximize and minimize the first Zagreb index among all trees with fixed number of vertices of degree two.

On the other hand, recall that a *segment* of a tree T [2, p. 219] is a path-subtree S whose terminal vertices are branching or pendent vertices of T (i.e., every internal vertex v of S has $d_T(v) = 2$). The number of the segments of a tree T is denoted by s_T. Dobrynin, Entringer and Gutman (Section 5 of [2]) summarized many applications of this concept for the calculation of the Wiener index (the sum of the distances between all pairs of vertices in a graph) of trees . This provokes one to state the following problem.

Problem B. Characterize the trees which maximize and minimize the first Zagreb index among all trees with fixed number of segments.

The aim of this paper is to give a complete solution of above problems. First, we need a simple observation.

Given a tree T, let $r = |V(T)| - |V_2(T)|$, then by squeezing out all vertices of degree 2 from T (i.e., replacing each segment of T by an edge), a $r-$vertex tree will remain, which we call the *squeeze* of T and denote by $S(T)$ (see Figure 1 for an example). Clearly, there is a bijection between the segments of T and the edges of $S(T)$. Thus

$$s_T = |E(S(T))| = |V(S(T))| - 1 = |V(T)| - |V_2(T)| - 1. \qquad (1)$$

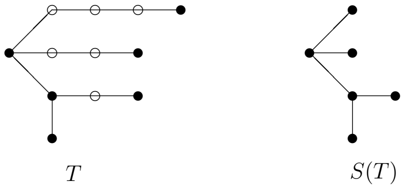
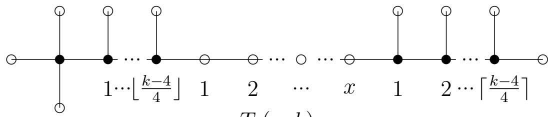


Fig. 1 A tree T and its squeeze $S(T)$

This observation follows that in an $n-$vertex tree T, s_T is determined by the number of vertices of degree two of T and vice versa.

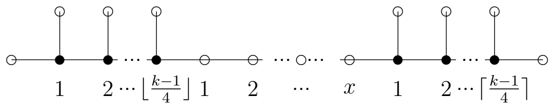
As usual, S_n and P_n denote, respectively, the star and path on n vertices. Denote by $\mathbb{ST}_{n,k}$ the set of all $n-$vertex trees with exactly k segments. Note that the path P_n is the unique element in $\mathbb{ST}_{n,1}$, the star S_n is the unique element in $\mathbb{ST}_{n,n-1}$ and the set $\mathbb{ST}_{n,2}$ is empty. So in the following we only consider the class $\mathbb{ST}_{n,k}$ with $3 \leq k \leq n-2$.

A tree is said to be *starlike of degree* k if exactly one of its vertices has degree greater than two, and this degree is equal to k, $k \geq 3$. A non-increasing sequence $\pi = (d_1, d_2, ..., d_n)$ is called *graphic* if there exists an $n-$vertex graph G such that $d_i = d_G(v)$ holds for some $v \in V(G)$. Given two positive integers n and k with $3 \leq k \leq n-2$, denote by $\mathbb{R}_{n,k}$ the set of all $n-$vertex starlike trees of degree k, by $\mathbb{O}_{n,k}$ the set of all $n-$vertex trees with the degree sequence $(\underbrace{3,...,3}_{\frac{k-1}{2}}, \underbrace{2,...,2}_{n-k-1}, \underbrace{1,...,1}_{\frac{k+3}{2}})$ for odd k and by $\mathbb{E}_{n,k}$ the set of all $n-$vertex trees with the degree sequence $(4, \underbrace{3,...,3}_{\frac{k-4}{2}}, \underbrace{2,...,2}_{n-k-1}, \underbrace{1,...,1}_{\frac{k+4}{2}})$ for even k. Clearly, each tree in $\mathbb{R}_{n,k}$ has the degree sequence $(k, \underbrace{2,...,2}_{n-k-1}, \underbrace{1,...,1}_{k})$. For any tree T in $\mathbb{R}_{n,k}$, $\mathbb{O}_{n,k}$ and $\mathbb{E}_{n,k}$, according to (1), $s_T = n - |V_2(T)| - 1 = n - (n-k-1) - 1 = k$, thus $\mathbb{R}_{n,k} \subseteq \mathbb{ST}_{n,k}$, $\mathbb{O}_{n,k} \subseteq \mathbb{ST}_{n,k}$ and $\mathbb{E}_{n,k} \subseteq \mathbb{ST}_{n,k}$. In Figure 2, we have drawn two specified trees $T_1(n,k) \in \mathbb{O}_{n,k}$ and $T_2(n,k) \in \mathbb{E}_{n,k}$.



$T_2(n,k)$

$x = n - k - 1$



$T_1(n,k)$

$x = n - k - 1$

Fig. 2 Two trees $T_1(n,k)$ and $T_2(n,k)$

Now we can state the main result of this paper.

Theorem 1. Let $T \in \mathbb{ST}_{n,k}$, where $3 \le k \le n-2$, then

$$4n + k^2 - 3k - 4 \ge M_1(T) \ge \begin{cases} 4n + k - 7 & \text{if } k \text{ is odd} \\ 4n + k - 4 & \text{if } k \text{ is even.} \end{cases}$$

The upper bound is attained if and only if $T \in \mathbb{R}_{n,k}$ and the lower bound is attained if and only if $T \in \mathbb{O}_{n,k}$ for odd k or $T \in \mathbb{E}_{n,k}$ for even k.

Remark 1. According to (1), Theorem 1 also characterizes the trees which maximize and minimize the first Zagreb index among all trees with fixed number of vertices of degree two.

The proof of the theorem is given in Section 3, while in Section 2 we provide some results to make the proof more compact.

2 Preliminaries

The following theorem due to Gutman and Das [5] is an elementary result on the first Zagreb index of trees.

Theorem 2 ([5]). Let T be a tree on n vertices, then

$$4n - 6 \le M_1(T) \le n(n-1).$$

The lower bound is attained if and only if $T \cong P_n$ and the upper bound is attained if and only if $T \cong S_n$.

A tree is called a *caterpillar* if the removal of all pendent vertices results in a path. Otherwise, it is called a *non-caterpillar*.

Lemma 3. Suppose T is an $n-$vertex non-caterpillar, then there exists an $n-$vertex caterpillar T' such that T' and T have the same degree sequence.

Proof. By construction. Let $r = |V_2(T)|$ and $k = |V_{\geq 3}(T)|$, then $|V_1(T)| = |V(T)| - |V_2(T)| - |V_{\geq 3}(T)| = n - k - r$. As T is a non-caterpillar, $k \geq 1$. We may assume that $\pi = (d_1, d_2, ..., d_n)$ is the degree sequence of T with

$d_1 \geq ... \geq d_k \geq 3 > d_{k+1} = ... = d_{k+r} = 2 > d_{k+r+1} = ... = d_n = 1.$

Since the relation $\sum\limits_{v \in V(G)} d_G(v) = 2|E(G)|$ (handshaking lemma) holds for any graph G, we have

$$(d_1 + d_2 + ... + d_k) + 2r + (n - k - r) = 2(n - 1). \tag{2}$$

Let R be the caterpillar (see Figure 3) obtained from a $(k + r + 1)-$vertex path $P = v_1 v_2 ... v_{k+r+1}$ by attaching t_i new vertices of degree one to each vertex v_i for $1 \leq i \leq k$ such that

$t_1 = d_1 - 1$, and if $k \geq 2$

$t_i = d_i - 2$ for each $i \in \{2, 3, ..., k\}$.

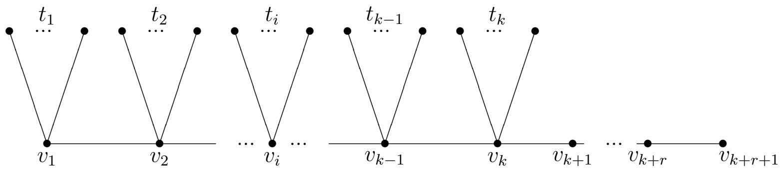


Fig. 3 The caterpillar R

Therefore,

$d_R(v_1) = d_1$, $d_R(v_2) = d_2$, ..., $d_R(v_k) = d_k$, and $d_R(v_{k+1}) = ... = d_R(v_{k+r}) = 2.$

Note that R has $t_1 + t_2 + ... + t_k + 1$ pendent vertices, by equation (2), we get

$t_1 + t_2 + ... + t_k + 1$

$= (d_1 - 1) + (d_2 - 2) + ... + (d_k - 2) + 1$

$= (d_1 + d_2 + ... + d_k) - 2k + 2$

$= 2(n-1) - 2r - (n-k-r) - 2k + 2$

$= n - k - r.$

Hence π also is the degree sequence of R. Now $T' = R$ is the desired tree. □

Lemma 4. Let T be a caterpillar and let $P = v_0v_1...v_lv_{l+1}$ be a longest path of T. Assume that there exists a vertex v_i ($1 \le i \le l$) such that $d_T(v_i) \ge 5$, suppose u and v ($u \ne v_0$, $u \ne v_{l+1}$, $v \ne v_0$ and $v \ne v_{l+1}$) are two pendent vertices adjacent to v_i. Let T' be the tree obtained from T by deleting the edges uv_i, vv_i and joining u and v to v_{l+1} (see Figure 4 for an example), then $M_1(T') < M_1(T)$.

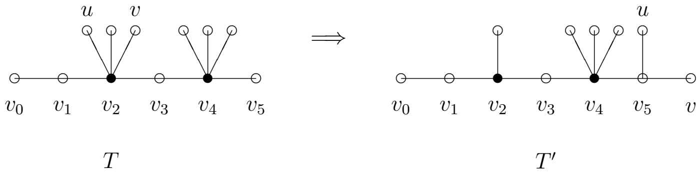


Fig. 4 Two caterpillars T and T'

Proof. We shall consider the difference $M_1(T) - M_1(T')$. Note that v_i and v_{l+1} are the only vertices whose degrees differ in T and T', $d_T(v_i) = d_{T'}(v_i) + 2$, $d_{T'}(v_{l+1}) = 3$ and $d_T(v_{l+1}) = 1$. Therefore,

$M_1(T) - M_1(T')$

$= [(d_T(v_i))^2 + (d_T(v_{l+1}))^2] - [(d_{T'}(v_i))^2 + (d_{T'}(v_{l+1}))^2]$

$= [(d_{T'}(v_i) + 2)^2 + 1] - [(d_{T'}(v_i))^2 + 9]$

$= 4d_{T'}(v_i) - 4$

≥ 8 (since $d_{T'}(v_i) = d_T(v_i) - 2 \ge 3$). □

Remark 2. For the trees T and T' described in Lemma 4, it is easy to see that $s_T = s_{T'}$. So if a caterpillar $T \in \mathbb{ST}_{n,k}$ contains a vertex of degree greater than 4, then by a transformation introduced in Lemma 4, one can get another caterpillar $T' \in \mathbb{ST}_{n,k}$ with $M_1(T') < M_1(T)$.

Lemma 5. Let T be a caterpillar and let $P = v_0v_1...v_lv_{l+1}$ be a longest path of T. Assume that there exists two vertices v_i and v_j ($1 \le i, j \le l$) such that $d_T(v_i) = d_T(v_j) = 4$, suppose u ($u \ne v_0$ and $u \ne v_{l+1}$) is a pendent vertex adjacent to v_i and v ($v \ne v_0$ and $v \ne v_{l+1}$) is a pendent vertex adjacent to v_j. Let T'' be the tree obtained from T by deleting the edges uv_i, vv_i and joining u and v to v_{l+1} (see Figure 5 for an example), then $M_1(T'') < M_1(T)$.

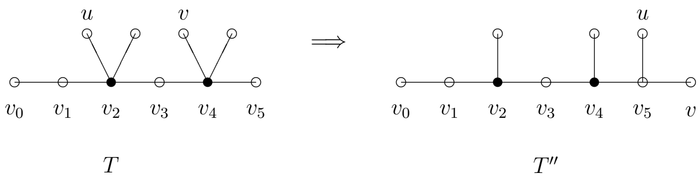


Fig. 5 Two caterpillars T and T''

Proof. We shall consider the difference $M_1(T) - M_1(T'')$. Note that v_i, v_j and v_{l+1} are the only vertices whose degrees differ in T and T''. Therefore,

$$\begin{aligned}
&M_1(T) - M_1(T'') \\
&= [(d_T(v_i))^2 + (d_T(v_j))^2 + (d_T(v_{l+1}))^2] - [(d_{T''}(v_i))^2 + (d_{T''}(v_j))^2 + (d_{T''}(v_{l+1}))^2] \\
&= [16 + 16 + 1] - [9 + 9 + 9] \\
&= 6. \quad \square
\end{aligned}$$

Remark 3. For the trees T and T'' described in Lemma 5, it is easy to see that $s_T = s_{T''}$. So if a caterpillar $T \in \mathbb{ST}_{n,k}$ contains two vertices of degree 4, then by a transformation introduced in Lemma 5, one can get another caterpillar $T'' \in \mathbb{ST}_{n,k}$ with $M_1(T'') < M_1(T)$.

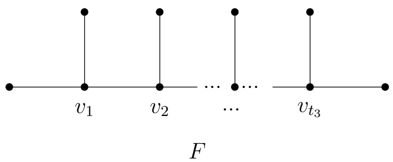


Fig. 6 The tree F

Lemma 6. Let T be a caterpillar with $\triangle(T) \leq 4$. Assume that T has t_3 vertices of degree 3 and t_4 vertices ($t_4 \leq 1$) of degree 4, then s_T is odd if $t_4 = 0$ and s_T is even if $t_4 = 1$.

Proof. Let F be the caterpillar as shown in Figure 6. When $t_4 = 0$, then $S(T) = F$, which follows that $s_T = s_F$ is odd. When $t_4 = 1$, then $S(T)$ can be obtained from F by adding a new vertex u and joining u to one vertex $v_i \in \{v_1, v_2, ..., v_{t_3}\}$, and thus $s_T = s_F + 1$ is even. $\square$

3 Proof of Theorem 1

Proof. By the definitions of the squeeze of a tree and the first Zagreb index, we have

$$M_1(T) = M_1(S(T)) + 4|V_2(T)|.$$

From (1), $|V_2(T)| = n - s_T - 1 = n - k - 1$, hence

$$M_1(T) = M_1(S(T)) + 4(n - k - 1).$$

Since $S(T)$ has $n - |V_2(T)| = k + 1$ vertices, by Theorem 2

$$M_1(S(T)) \leq k^2 + k,$$

with equality if and only if $S(T) = S_{k+1}$.

If $S(T) = S_{k+1}$, then $T \in \mathbb{R}_{n,k}$. So we arrive at

$$M_1(T) \leq k^2 + k + 4(n - k - 1) = 4n + k^2 - 3k - 4,$$

with equality if and only if $T \in \mathbb{R}_{n,k}$.

Now we turn to determine the lower bound of $M_1(T)$. Let T^* be a tree with the minimal Zagreb index in $\mathbb{ST}_{n,k}$ and let π be its degree sequence.

By Lemma 3, we can always find a caterpillar $T_c^* \in \mathbb{ST}_{n,k}$ with π as its degree sequence (if T^* is a caterpillar, we may set $T_c^* = T^*$). Consequently,

$$M_1(T^*) = M_1(T_c^*).$$

Claim 1. $\triangle(T_c^*) \leq 4$.

Suppose, to the contrary, $\triangle(T_c^*) \geq 5$, then by a transformation described in Lemma 4, we can get a caterpillar $T' \in \mathbb{ST}_{n,k}$ with $M_1(T') < M_1(T_c^*) = M_1(T^*)$, contradicting to the minimality of T^*.

Claim 2. T_c^* has at most one vertex of degree 4.

Suppose, to the contrary, T_c^* has at least two vertices of degree 4, then by a transformation introduced in Lemma 5, we can get a caterpillar $T'' \in \mathbb{ST}_{n,k}$ with $M_1(T'') < M_1(T_c^*) = M_1(T^*)$, contradicting to the minimality of T^*.

Now we can conclude that T_c^* should possess only vertices of degree 1, 2, 3 and at most one vertex of degree 4. For each $i \in \{1, 2, 3, 4\}$, let t_i denote the number of its vertices of degree i. To obtain exact value of $M_1(T_c^*)$, we shall examine two cases.

Case 1. k is odd.

In this case, according to Lemma 6, $t_4 = 0$. From (1),

$$t_2 = n - k - 1. \tag{3}$$

Since T_c^* is a caterpillar, it is easy to see that

$$t_1 = t_3 + 2. \tag{4}$$

From handshaking lemma,

$$t_1 + 2t_2 + 3t_3 = 2n - 2. \tag{5}$$

Combining (3), (4) and (5), we get

$$t_1 = \tfrac{k+3}{2} \quad \text{and} \quad t_3 = \tfrac{k-1}{2},$$

which lead to

$$\pi = (\underbrace{3, ..., 3}_{\frac{k-1}{2}}, \underbrace{2, ..., 2}_{n-k-1}, \underbrace{1, ..., 1}_{\frac{k+3}{2}}).$$

Hence $T^* \in \mathbb{O}_{n,k}$, and

$$M_1(T^*) = 9(\tfrac{k-1}{2}) + 4(n-k-1) + \tfrac{k+3}{2} = 4n + k - 7.$$

Case 2. k is even.

In this case, according to Lemma 6, $t_4 = 1$. From (1),

$$t_2 = n - k - 1. \tag{6}$$

Since T_c^* is a caterpillar, it is easily checked that

$$t_1 = t_3 + 2t_4 + 2 = t_3 + 4, \tag{7}$$

From handshaking lemma,

$$t_1 + 2t_2 + 3t_3 + 4t_4 = t_1 + 2t_2 + 3t_3 + 4 = 2n - 2. \tag{8}$$

Combining (6), (7) and (8), we obtain

$$t_1 = \tfrac{k+4}{2} \quad \text{and} \quad t_3 = \tfrac{k-4}{2},$$

which lead to

$$\pi = (4, \underbrace{3, ..., 3}_{\frac{k-4}{2}}, \underbrace{2, ..., 2}_{n-k-1}, \underbrace{1, ..., 1}_{\frac{k+4}{2}}).$$

Hence $T^* \in \mathbb{E}_{n,k}$, and

$$M_1(T^*) = 16 + 9(\tfrac{k-4}{2}) + 4(n-k-1) + \tfrac{k+4}{2} = 4n + k - 4,$$

by which the proof of Theorem 1 is completed. □

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