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Second Zagreb Index of Trees with Fixed Diameter

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Abstract: Let G be a simple graph with vertex set $V = V(G) = \{v_1, v_2, ..., v_n\}$ and edge set $E = E(G)$. For $v_i \in V(G)$, by $d_i = d_i(G)$ we denote the degree (number of neighbors) of the vertex v_i. The second Zagreb index is defined as $M_2(G) = \sum\limits_{v_i v_j \in E(G)} d_i d_j$. In this paper, we study the minimal and maximal second Zagreb index of trees with fixed diameter.

Keywords: second Zagreb index, diameter, trees

1 Introduction

We recall some terminologies in graph theory from [1]. Let G be a simple graph with vertex set $V = V(G) = \{v_1, v_2, ..., v_n\}$ and edge set $E = E(G)$. For $v_i \in V(G)$, by $d_i = d_i(G)$ we denote the degree (number of neighbors) of the vertex v_i. For any two distinct vertices u and v in G, the distance between u and v, denoted by $d_G(u, v)$, is the number of edges in a shortest path joining u and v. The diameter d of G is the maximum distance between any two vertices of G. Let S_n and P_n be a star and a path on n vertices, respectively.

The second Zagreb index is defined as

$$M_2(G) = \sum_{v_i v_j \in E(G)} d_i d_j.$$

The second Zagreb index is one of the oldest vertex-degree-based molecular structure descriptors, invented in the 1970s [9, 10]. Details of its theory can be found in the recent review [2] and the recent papers [5, 3, 4] whereas data on their history in [8].

Researching in the field of vertex-degree-based topological indices with given diameter is one of the attractive topics in the chemical graph theory. Well known Wiener index of a graph G is defined by

$$W(G) = \sum_{v_i v_j \in E(G)} d(v_i, v_j).$$

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Recently, Sun et al. in the paper [11] provides some new results about maximal values of $W(G)$ with given diameter. In the paper [13], Liu and Pan obtained some results on Wiener index of trees with fixed diameter.

The Hararay index of a graph G is defined as

$$H(G) = \sum_{\{u,v\} \subset V(G)} \frac{1}{d(u,v)}.$$

In the the paper [6], Feng et al. obtained trees with minimal value of $H(G)$ with fixed diameter 3 and 4.

Inspired by the paper [6] we consider second Zagreb index of trees which have minimal and maximal values with fixed diameter 3 and 4. We will also compare our results with the upper bound from [12]

$$M_2(G) \leq \frac{1}{2}(m^2 - m(d-3) + (d-2))\sqrt{2m-n+1}. \tag{1}$$

2 Main results

Let $\mathscr{T}_{n,d}$ be the set of trees of order n and diameter d. In the class $\mathscr{T}_{n,2}$ there is only one graph which is star S_n. The trees in $\mathscr{T}_{n,3}$ are obtained from a path $P_4 = v_1v_2v_3v_4$ by attaching a pendant vertices at v_2 and b pendant vertices at v_3. We will denote this tree by $T_3(a,b)$ (Figure 1).

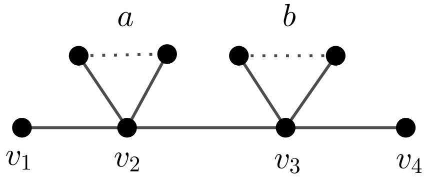

Fig. 1. $T_3(a,b)$

Theorem 2.1. *For $T_3(a,b) \in \mathscr{T}_{n,3}$, we have*

$$M_2(T_3(a,b)) \geq \begin{cases} \frac{3}{4}n^2 - n, & \text{if } n \text{ is even} \\ \frac{3}{4}n^2 - n + \frac{1}{4}, & \text{if } n \text{ is odd.} \end{cases}$$

The equality holds if and only if $a = \frac{n-4}{2}$ when n is even or $a = \frac{n-3}{2}$ or $a = \frac{n-5}{2}$ when n is odd.

Proof. Bearing in mind that $a+b=n-4$ and using Figure 1, we have

$$\begin{aligned} M_2(T_3(a,b)) &= a+2+a(a+2)+(a+2)(b+2)+b(b+2)+b+2 \\ &= 5(a+b)+(a+b)^2-ab+8 \\ &= a^2-(n-4)a+n^2-3n+4 \end{aligned}$$

It follows that

$$M_2(T_3(a,b)) = \left(a-\frac{n-4}{2}\right)^2 - \frac{(n-4)^2}{4} + n^2-3n+4. \tag{2}$$

If n is even, then the minimal value of (2) is attained for $a=\frac{n-4}{2}$ and we have

$$M_2(T_3(a,b)) \geq \frac{3}{4}n^2-n.$$

If n is odd, then the minimal value of (2) is attained for $a=\frac{n-3}{2}$ or $a=\frac{n-5}{2}$ and we get

$$M_2(T_3(a,b)) \geq \frac{3}{4}n^2-n+\frac{1}{4}.$$

□

Now, we are going to find trees with maximal value of M_2 in the class $\mathscr{T}_{n,3}$.

Theorem 2.2. *(a) If $b \geq a$, then $M_2(T_3(a,b)) < M_2(T_3(a-1,b+1))$.*

(b) If $b < a$, then $M_2(T_3(a,b)) < M_2(T_3(a+1,b-1))$.

Proof. Claims (a) and (b) follow from (2) and

$$M_2(T_3(a-1,b+1)) = a^2+b^2+ab+4a+6b+9,$$

$$M_2(T_3(a+1,b-1)) = a^2+b^2+ab+6a+4b+9.$$

□

Remark 2.1. *By the theorem 2.2, for $T \in \mathscr{T}_{n,3}$ it follows*

$$M_2(T) \leq n^2-3n+4, \tag{3}$$

with equality if and only if $T \cong T_3(0,n-4)$ or $T \cong T_3(n-4,0)$.

Remark 2.2. *For $d=3$ and $m=n-1$ in (1) we obtain*

$$M_2(G) \leq \frac{1}{2}(n^2-2n+2)\sqrt{n-1} \tag{4}$$

The upper bound (3) is better than the upper bound (4).

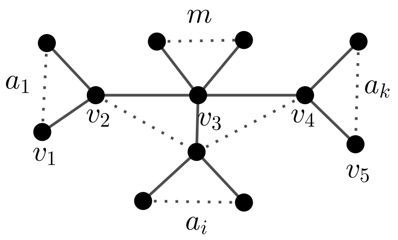

Fig. 2. $T_4(m;a_1,a_2,...,a_k)$

Next, we consider the trees with diameter 4. Let $\mathscr{T}_{n,4}$ be a class of trees with n vertices and diameter $d=4$. The trees in $\mathscr{T}_{n,4}$ are of the form like $T_4(m;a_1,a_2,...,a_k)$ with $m \geq 0$, as shown in figure 2, where $\sum\limits_{i=1}^{k} a_i+m+k+1=n$. The tree $T_4(m;a_1,a_2,...,a_k)$ is obtained from a path $P_5=v_1v_2v_3v_4v_5$ by attaching some pendant edges at v_2, v_4, and/or attaching some pendant edges at v_3, and/or identifying v_3 with a pendant vertex of a star. If $m=0$ we will write $T_4(a_1,a_2,...,a_k)$ instead $T_4(m;a_1,a_2,...,a_k)$.

Theorem 2.3. *For any tree of order $n \geq 16$ of the form $\tilde{T}=T_4(m;a_1,a_2,...,a_k) \in \mathscr{T}_{n,4}$, where $k \geq 2, m \geq 1$, there exists a tree of order $n \geq 16$ of the form $T=T_4(b_1,b_2,...,b_t)$ such that $M_2(\tilde{T}) \geq M_2(T)$.*

Proof. Let $k \geq 2, m \geq 1$ and without loss of generality we assume $a_1 \leq a_2 \leq \cdots \leq a_k$. Let $T'=T(m-1;a_1+1,a_2,...,a_k)$. Now we have

$$M_2(\tilde{T})=\sum_{i=1}^{k}(m+3)(a_i+1)+\sum_{i=1}^{k}a_i(a_i+1)+m(m+3), \tag{5}$$

$$\begin{aligned} M_2(T') &= \sum_{i=2}^{k}(m+2)(a_i+1)+(a_1+2)(m+2) \\ &\quad +\sum_{i=2}^{k}a_i(a_i+1)+(a_1+1)(a_1+2)+(m-1)(m+2) \end{aligned} \tag{6}$$

$$\begin{aligned} M_2(\tilde{T})-M_2(T') &= (m+2)\sum_{i=2}^{k}(a_i+1)+(m+2)(a_1+1)+\sum_{i=1}^{k}(a_i+1)+\sum_{i=2}^{k}a_i(a_i+1) \\ &+ a_1(a_1+1)+m(m+3) \\ &- (m+2)\sum_{i=2}^{k}(a_i+1)-(a_1+2)(m+2)-\sum_{i=2}^{k}a_i(a_i+1) \\ &- (a_1+1)(a_1+2)-(m-1)(m+2) \\ &= \sum_{i=1}^{k}a_i+k+m-2a_1-2 \geq 0. \end{aligned}$$

The last inequality holds because $k \geq 2$, $\sum_{i=1}^{k} a_i \geq ka_1 \geq 2a_1$ and $m \geq 1 > 0$. $\square$

Remark 2.3. *From the Theorem 2.3, one can see that tree with minimal value of M_2 is of the form $T_4(a_1, a_2, ..., a_k)$ and it holds that $n-1-k \geq k$, i.e., $k \leq \frac{n-1}{2}$.*

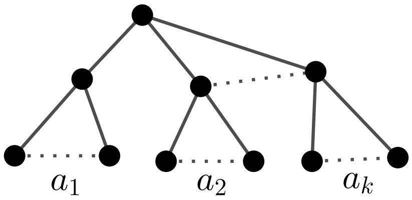

Fig. 3. $T_4(a_1, a_2, ..., a_k)$

Theorem 2.4. *Let $T = T_4(a_1, a_2, ..., a_k)$ be the tree of order n with diameter 4 and $k \geq 2$ as depicted in Figure 3. Then we have*

$$M_2(T) = (n-1)k + n - 1. \tag{7}$$

Proof. Since $m = 0$ and $\sum_{i=1}^{k} a_i = n-k-1$, we have

$$M_2(T) = \sum_{i=1}^{k}(a_i+1) + \sum_{i=1}^{k} k(a_i+1) = (k+1)\sum_{i=1}^{k}(a_i+1) = (n-1)k + n - 1.$$

$\square$

Remark 2.4. *Since $k \geq 2$, one can see that (7) is minimized for $k = 2$. By theorems 2.3 and 2.4, for $T \in \mathscr{T}_{n,4}$ it follows that*

$$M_2(T) \geq M_2(T(a_1, a_2, 0, ..., 0)).$$

Next, we consider the trees form the class $\mathscr{T}_{n,4}$ which have maximal value of M_2.

Theorem 2.5. $M_2(T_4(m; a_1, a_2, ..., a_k)) < M_2(T_4(m+1; a_1-1, a_2, ..., a_k))$.

Proof. Using the right-hand side of (5) and

$$\begin{aligned} M_2(T_4(m+1; a_1-1, a_2, ..., a_k)) &= \sum_{i=2}^{k}(m+4)(a_i+1) + (m+4)a_1 \\ &+ \sum_{i=2}^{k} a_i(a_i+1) + (a_1-1)\cdot a_1 + (m+1)(m+4), \end{aligned}$$

we have

$$M_2(T_4(m+1; a_1-1, a_2, ..., a_k)) - M_2(T_4(m; a_1, a_2, ..., a_k) > 0.$$

$\square$

Remark 2.5. *By the Theorem 2.5 one can see that for* $T \in \mathscr{T}_{n,4}$ *we have*

$$M_2(T) \leq n^2 - 4n + 7, \tag{8}$$

with equality if and only if $T \cong T_4(n-k-3;1,0,0,...,1)$. *Notice that*

$$\begin{aligned} M_2(T_4(n-k-3;1,0,0,...,0,1)) &= M_2(T_4(n-k-3;0,1,0,...,0,1)) \\ &= \cdots = M_2(T_4(n-k-3;0,0,0,...,1,1)). \end{aligned}$$

Remark 2.6. *For* $d = 4$ *and* $m = n-1$ *in (1) we obtain*

$$M_2(G) \leq \frac{1}{2}(n-1)(n-2)\sqrt{n-1} + \sqrt{n-1}. \tag{9}$$

The upper bound (8) is better than the upper bound (9).

References

[1] C. Berge, *Graphs*, North-Holland, Amsterdam, 1985.

[2] B. Borovićanin, B. Furtula, K. C. Das, I. Gutman, *Zagreb indices: bounds and extremal graphs*, in: I. Gutman, B. Furtula, K. C. Das, I. Ž Milovanović, E. I. Milovanović, Bounds in Chemical Graph Theory - Basics, Univ. Kragujevac, Kragujevac, 2017, pp. 67-153.

[3] B. Borovićanin, T. Aleksić Lampert, O*n the Maximum and Minimum Zagreb Indices of Trees with a Given Number of Vertices of Maximum Degree*, MATCH Commun. Math. Comput. Chem. 74 (2015), 81-96.

[4] B. Borovićanin, *On the Extremal Zagreb Indices of Trees with Given Number of Segments or Given Number of Branching Vertices*, MATCH Commun. Math. Comput. Chem. 74 (2015), 57-79.

[5] K. C. Das, K. Xu, I. Gutman, *On Zagreb and Harary indices*, MATCH Commun. Math. Comput. Chem. 70 (2013), 301-314.

[6] L. Feng, Y. Lan, W. Liu, X. Wang, *Minimal Harary Index of Graphs with Small Parameters*, MATCH Commun. Math. Comput. Chem. 76 (2016), 23-42.

[7] I. Gutman, *Graphs with smallest sum of squares of vertex degrees*, Kragujevac J. Math. 25 (2003), 51-54.

[8] I. Gutman, *On the origin of two degree-based topological indices*, Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.) 146 (2014), 39-52.

[9] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, *Graph theory and molecular orbitals. XII. Acyclic polyenes*, J. Chem. Phys. 62 (1975), 3399-3405.

[10] I. Gutman, N. Trinajstić, *Graph theory and molecular orbitals. Total* π*-electron energy of alternant hydrocarbon*, Chem. Phys. Lett. 17 (1972), 535-538.

[11] Q. Sun, B. Ikica, R. Škrekovski, V. Vukašinović, *Graphs with a given diameter that maximise the Wiener index*, Appl. Math. Comput. 356 (2019), 438-448.

[12] B. LIU, I. GUTMAN, *Upper bounds for Zagreb indices of connected graphs*, MATCH Commun. Math. Comput. Chem. 55 (2006), 439-446.

[13] H. LIU, X. PAN, *On the Wiener Index of Trees with Fixed Diameter*, MATCH Commun. Math. Comput. Chem. 60 (2008), 85-94.