

An Upper Bound on the First Zagreb Index in Trees

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ABSTRACT

The first Zagreb index $M_1(G)$ is equal to the sum of squares of the degrees of the vertices and the first Zagreb coindex $\overline{M}_1(G)$ is equal to the sum of sums of vertex degrees of the pairs of non-adjacent vertices. Kovijanić Vukićević and G. Popivoda (Iran. J. Math. Chem. 5 (2014) 19–29) proved that for any chemical tree of order n , $n \geq 5$,

$$M_1(T) \leq \begin{cases} 6n - 12 & n \equiv 0, 1 \pmod{3} \\ 6n - 10 & \text{otherwise.} \end{cases}$$

In this paper, we generalize the aforementioned bound for all trees in terms of their order and maximum degree. Moreover, we give a lower bound on the first Zagreb coindex of trees.

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1. INTRODUCTION

In this paper, G is a simple connected graph with vertex set $V = V(G)$ and edge set $E = E(G)$. The order $|V|$ of G is denoted by $n = n(G)$. For every vertex $v \in V$, the *open neighborhood* $N(v)$ is the set $\{u \in V(G) \mid uv \in E(G)\}$ and the *closed neighborhood* of v is the set $N[v] = N(v) \cup \{v\}$. The *degree* of a vertex $v \in V$ is $d_v = |N(v)|$. The *minimum* and *maximum degree* of a graph G are denoted by $\delta = \delta(G)$ and $\Delta = \Delta(G)$, respectively. Trees with the property $\Delta \leq 4$ are called chemical trees.

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajestić in [6]. They are important molecular descriptors and have been closely correlated with many chemical properties [6, 7]. Thus, it attracted more and more attention from chemists and mathematicians [2, 3, 4, 8, 10, 11].

The *first Zagreb index* $M_1(G)$ is defined as follows:

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$$M_1(G) = \sum_{v \in V} d_v^2.$$

The first Zagreb index can be also expressed as the sum of vertex degree over edges of G , that is, $M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$. Došlić in [5] introduced a new graph invariant called the *first Zagreb coindex*, as $\overline{M}_1(G) = \sum_{uv \notin E(G)} (d_u + d_v)$. Next we introduce a family of trees. For $n = (\Delta - 1)k + p$ ($k \geq 2$), let \mathbb{T}_n be the family of trees of order n with maximum degree Δ such that:

- If $p = 0$, $k - 1$ vertices have degree Δ , 1 vertex has degree $\Delta - 2$ and remaining vertices are pendant.
- If $p = 1$, $k - 1$ vertices have degree Δ , 1 vertex has degree $\Delta - 1$ and remaining vertices are pendant.
- If $p = 2$, k vertices have degree Δ and remaining vertices are pendant.
- If $p \geq 3$, k vertices have degree Δ , 1 vertex has degree $p - 1$, and $n - k - 1$ remaining vertices are pendant.

Kovijanić Vukićević and Popivoda [9] proved the following upper bound on the first Zagreb index of chemical trees and characterized all extreme chemical trees.

Theorem 1. Let T be a chemical tree with $n \geq 5$ vertices. Then

$$M_1(T) \leq \begin{cases} 6n - 12 & n \equiv 0, 1 \pmod{3} \\ 6n - 10 & \text{otherwise,} \end{cases}$$

with equality if and only if $G \in \mathbb{T}_n$.

In this paper, we establish an upper bound on the first Zagreb index of trees in terms of the order and maximum degree, as a generalization of aforementioned bound. As a consequence, we obtain a lower bound on the first Zagreb coindex for trees.

2. MAIN RESULTS

In this section, we prove the following result:

Theorem 2. Let T be a tree of order n and maximum degree Δ . If $n \equiv p \pmod{\Delta - 1}$, then

$$M_1(T) \leq \begin{cases} (\Delta + 2)n - 4\Delta + 4 & p = 0 \\ (\Delta + 2)n - 3\Delta & p = 1 \\ (\Delta + 2)n - 2\Delta - 2 & p = 2 \\ (\Delta + 2)n - 2\Delta - 3 + p(p - 2) & p \geq 3, \end{cases}$$

with equality if and only if $G \in \mathbb{T}_n$.

To prove Theorem 2, we proceed with some definitions and lemmas. If n is a positive integer, then an integer partition of n is a non-increasing sequence of positive integers (a_1, a_2, \dots, a_t) whose sum is n . If $1 \leq a_1 \leq a_2 \leq \dots \leq a_t \leq a$, then (a_1, a_2, \dots, a_t) is called an integer partition of n on $N_a = \{1, 2, \dots, a\}$. An integer partition (a_1, a_2, \dots, a_t) of n on N_a is called an integer a -partition if the number of a in this partition is as large as possible. In other words, if $n = ka$, then (a, \dots, a) is the integer a -partition and if $n = ka + b$ where $0 < b < a$ then (b, a, \dots, a) is the integer a -partition. The proof of the next result is straightforward and therefore omitted.

Lemma 3. For positive integers n, t and a_i ($1 \leq i \leq t$), we have

- a) If $n = a_1 + a_2 + \dots + a_t$ and $t > 1$, then $n^2 > a_1^2 + a_2^2 + \dots + a_t^2$.
- b) If $a_i \leq a_j$, then $(a_i - 1)^2 + (a_j + 1)^2 \geq a_i^2 + a_j^2 + 2$.

Lemma 4. If (a_1, a_2, \dots, a_t) is an integer partition of $n = ka + b$ ($0 \leq b < a$) on N_a , then

$$\sum_{i=1}^t a_i^2 < ka^2 + b^2.$$

Proof. Let (a_1, a_2, \dots, a_t) be an partition of n on N_a . If $a_i \leq a_j < a$ for some $1 \leq i \neq j \leq t$, then by switching (a_i, a_j) to $(a_i - 1, a_j + 1)$, we get a new integer partition of n on N_a . Note that if $a_i - 1 = 0$, then we will remove $a_i - 1$ from the new partition. Applying Lemma 3 (a), we obtain

$$\sum_{i=1}^t a_i^2 < a_1^2 + \dots + (a_i - 1)^2 + \dots + (a_j + 1)^2 + \dots + a_t^2.$$

By repeating this process, we arrive at an integer a -partition of n on N_a . It follows from Lemma 2 that $\sum_{i=1}^t a_i^2 < ka^2 + b^2$ and the proof is complete.

Lemma 5. Let $n = ka + b$ where $0 \leq b < a$ and let (a_1, a_2, \dots, a_t) be an integer partition of n on N_a which is not a -partition. Then the following statements holds:

- a. If $b > 0$, then $\sum_{i=1}^t (a_i + 1)^2 < k(a + 1)^2 + (b + 1)^2$.
- b. If $b = 0$, then $\sum_{i=1}^t (a_i + 1)^2 < k(a + 1)^2$.

Proof. (a) Since $n = a_1 + \dots + a_t = b + \underbrace{a + \dots + a}_k = ka + b$, we have $t \geq k + 1$. First let $t = k + 1$. Then we have

$$\begin{aligned} (a_1 + 1)^2 + \dots + (a_t + 1)^2 &= (a_1^2 + \dots + a_t^2) + t + 2(ka + b) \\ &< (ka^2 + b^2) + t + 2(ka + b) \quad (\text{by Lemma 3}) \\ &= k(a + 1)^2 + (b + 1)^2 + t - (k + 1) \\ &= k(a + 1)^2 + (b + 1)^2, \end{aligned}$$

as desired. Now let $t > k + 1$. Repeating the switching process described in the proof of Lemma 4, i.e. for any pair (a_i, a_j) where $1 \leq a_i < a_j < a$ and using the fact that $a_i^2 + a_j^2 \leq (a_i - 1)^2 + (a_j + 1)^2 - 2$, we get $a_i = 0$ or $a_j = a$. To achieving an integer a -partition, we need to apply the switching process at least $t - (k + 1)$ times. This implies that

$$a_1^2 + \dots + a_t^2 \leq ka^2 + b^2 - 2(t - (k + 1)). \quad (1)$$

Thus

$$\begin{aligned} (a_1 + 1)^2 + \dots + (a_t + 1)^2 &= (a_1^2 + \dots + a_t^2) + t + 2(ka + b) \\ &\leq ka^2 + b^2 - 2(t - (k + 1)) + t + 2(ka + b) \quad (\text{by inequality (1)}) \\ &= k(a + 1)^2 + (b + 1)^2 - (t - (k + 1)) \\ &< k(a + 1)^2 + (b + 1)^2. \end{aligned}$$

(b) If $b = 0$, then $n = a_1 + \dots + a_t = \underbrace{a + \dots + a}_k = ka$. Since (a_1, \dots, a_t) is not a -partition, we have $t > k$. Applying (1), we obtain

$$\begin{aligned} (a_1 + 1)^2 + \dots + (a_t + 1)^2 &= (a_1^2 + \dots + a_t^2) + t + 2ka \\ &\leq ka^2 - 2(t - k) + t + 2ka \\ &= k(a + 1)^2 + k - t \\ &< k(a + 1)^2. \end{aligned}$$

This completes the proof.

Remark 6. Let T be a tree of order n and maximum degree Δ . For each $i \in \{1, 2, \dots, \Delta\}$, let n_i denote the number of vertices of degree i . Then

$$n_1 + n_2 + \dots + n_\Delta = n \tag{2}$$

and

$$n_1 + 2n_2 + \dots + \Delta n_\Delta = 2n - 2. \tag{3}$$

Subtracting (2) from (3), yields

$$n_2 + 2n_3 + \dots + (\Delta - 1)n_\Delta = n - 2. \tag{4}$$

By (4), we obtain the following integer partition

$$\underbrace{(1, \dots, 1)}_{n_2}, \underbrace{(2, \dots, 2)}_{n_3}, \dots, \underbrace{(\Delta - 1, \dots, \Delta - 1)}_{n_\Delta}, \tag{5}$$

of $n - 2$ on $N_{\Delta-1} = \{1, 2, \dots, \Delta - 1\}$. It follows from Lemma 4 that $2^2 n_2 + 3^2 n_3 + \dots + \Delta^2 n_\Delta$ is maximum if and only if the partition (5) obtained from (4), is an $(\Delta - 1)$ -partition of $n - 2$ on $N_{\Delta-1}$. In that case, n_1 (the number of leaves) will be maximum.

Next result is an immediate consequence of above discussion.

Corollary 7. For any tree T of order n with maximum degree Δ , the first Zagreb index $M_1(T) = n_1 + 2^2 n_2 + \dots + \Delta^2 n_\Delta$ is maximum if and only if the integer partition (5) is an $(\Delta - 1)$ -partition of $n - 2$ on $N_{\Delta-1}$. In that case, the integer partition $(n_1, n_2, \dots, n_\Delta)$ is called an optimal solution of (4).

Theorem 8. Let T be a tree of order n and maximum degree Δ with $n \equiv 0 \pmod{\Delta - 1}$. Then $M_1(T) \leq (\Delta + 2)n - 4\Delta + 4$, with equality if and only if $T \in \mathbb{T}_n$.

Proof. Assume that $n = (\Delta - 1)k$. By (4),

$$n_\Delta = k - \left(\frac{n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} + 2}{\Delta - 1} \right) = k - r,$$

where $r = \frac{n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} + 2}{\Delta - 1}$. Then $1 \leq r \leq k - 1$ and $1 \leq n_\Delta \leq k - 1$. We

consider three cases as follows:

Case 1. $r = 1$. Then clearly $n_\Delta = k - 1$. It follows that

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} + (\Delta - 1)(k - 1) = (\Delta - 1)k - 2$$

and so

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = \Delta - 3.$$

Thus $n_{\Delta-1} = 0$ and so

$$n_2 + 2n_3 + \dots + (\Delta - 3)n_{\Delta-2} = \Delta - 3. \quad (6)$$

According to Corollary 6, the optimal solution of (6) is $n_2 = n_3 = \dots = n_{\Delta-3} = 0$ and $n_{\Delta-2} = 1$. Since $n_1 + n_2 + \dots + n_{\Delta} = n$, we conclude that $n_1 = (\Delta - 2)k$. By Corollary 7,

$$(n_1, n_2, \dots, n_{\Delta-3}, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k, 0, \dots, 0, 1, 0, k - 1)$$

is the optimal solution and so $M_1(T)$ is maximum. Therefore,

$$\begin{aligned} M_1(T) &\leq n_1 + 2^2 n_2 + \dots + (\Delta - 2)^2 n_{\Delta-2} + (\Delta - 1)^2 n_{\Delta-1} + \Delta^2 n_{\Delta} \\ &= (\Delta - 2)k + (\Delta - 2)^2 + \Delta^2(k - 1) \\ &= (\Delta + 2)(\Delta - 1)k - 4\Delta + 4 \\ &= (\Delta + 2)n - 4\Delta + 4. \end{aligned}$$

Case 2. $2 \leq r < \Delta$. Then $n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)r + (r - 2)$. Since $r - 2 < \Delta - 2$, it follows from Corollary 7 that

$$(n_1, n_2, \dots, n_{r-2}, n_{r-1}, n_r, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k - 1, 0, \dots, 0, 1, 0, \dots, 0, r, k - r)$$

is an optimal solution in this case. Since $2 \leq r < \Delta$ and $4 \leq \Delta$, we have $r(r - 2\Delta - 1) < -4\Delta + 4$ and so

$$\begin{aligned} M_1(T) &\leq (\Delta - 2)k - 1 + (r - 1)^2 + (\Delta - 1)^2 r + \Delta^2(k - r) \\ &= (\Delta + 2)(\Delta - 1)k + r(r - 2\Delta - 1) \\ &< (\Delta + 2)n - 4\Delta + 4. \end{aligned}$$

Case 3. $\Delta \leq r \leq k - 1$. Then $n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)r + (r - 2)$. There are non-negative integers t, s such that $(r - 2) = t(\Delta - 2) + s$ and $0 \leq s < \Delta - 2$. Hence $n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)(r + t) + s$. If $0 < s < \Delta - 2$, then

$$(n_1, n_2, \dots, n_s, n_{s+1}, n_{s+2}, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k - (t + 1), 0, \dots, 0, 1, 0, \dots, 0, r + t, k - r)$$

is the optimal solution and since $(s - \Delta) < 0$ and $4 \leq \Delta \leq r$, we obtain

$$\begin{aligned} M_1(T) &\leq (\Delta - 2)k - (t + 1) + (s + 1)^2 + (\Delta - 1)^2(r + t) + \Delta^2(k - r) \\ &= (\Delta + 2)(\Delta - 1)k + s(s + 2) + r(1 - 2\Delta) + t\Delta(\Delta - 2) \\ &= (\Delta + 2)n + (s - \Delta)(s + 2) - r\Delta + r \\ &< (\Delta + 2)n + (s - \Delta)(s + 2) - r\Delta + r \\ &< (\Delta + 2)n - 4\Delta + 4. \end{aligned}$$

If $s = 0$, then the optimal solution is

$$(n_1, n_2, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k - t, 0, \dots, 0, r + t, k - r).$$

Since $t(\Delta - 2) = r - 2 - s$, $(s + 2) > 0$ and $4 \leq \Delta \leq r$, we conclude that

$$\begin{aligned} M_1(T) &\leq n_1 + 4n_2 + 9n_3 + \dots + \Delta^2 \cdot n_\Delta \\ &= ((\Delta - 2)k - t) + (\Delta - 1)^2(r + t) + \Delta^2(k - r) \\ &= \Delta k - 2k - t + \Delta^2 r - 2\Delta r + r + \Delta^2 t - 2\Delta t + t + \Delta^2 k - \Delta^2 r \\ &= (\Delta + 2)n - (s + 2) - r\Delta + r \\ &< (\Delta + 2)n - r\Delta + r \\ &< (\Delta + 2)n - 4\Delta + 4. \end{aligned}$$

Therefore, in all cases $M_1(T) \leq (\Delta + 2)n - 4\Delta + 4$. If $T \in \mathbb{T}_n$, then clearly $M_1(T) = (\Delta + 2)n - 4\Delta + 4$. Conversely, let T be a tree of order n with $n \equiv 0 \pmod{\Delta - 1}$ and $M_1(T) = (\Delta + 2)n - 4\Delta + 4$. This occurs only in Case 1, that is, T has $k - 1 = \frac{n - \Delta + 1}{\Delta - 1}$ vertices of degree Δ , one vertex of degree $\Delta - 2$ and $(\Delta - 2)k$ leaves. Hence $T \in \mathbb{T}_n$ and the proof is complete.

Theorem 9. Let T be a tree of order n with maximum degree Δ and $n \equiv 1 \pmod{\Delta - 1}$. Then $M_1(T) \leq (\Delta + 2)n - 3\Delta$, with equality if and only if $T \in \mathbb{T}_n$.

Proof. Let $n = (\Delta - 1)k + 1$. Set $r = \frac{n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} + 1}{\Delta - 1}$. By (4),

$$n_\Delta = k - \left(\frac{n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} + 1}{\Delta - 1} \right) = k - r.$$

Then clearly $1 \leq r \leq k - 1$ and $1 \leq n_\Delta \leq k - 1$. We consider three cases.

Case 1. $r = 1$. Since $n_\Delta = k - 1$, it follows from (4) that $n_2 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)$ and by Corollary 7

$$(n_1, n_2, \dots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta - 2)k + 1, 0, \dots, 0, 1, k - 1)$$

is the optimal solution. Thus

$$\begin{aligned} M_1(T) &\leq n_1 + 2^2 n_2 + \dots + (\Delta - 2)^2 \cdot n_{\Delta-2} + (\Delta - 1)^2 \cdot n_{\Delta-1} + \Delta^2 \cdot n_\Delta \\ &= ((\Delta - 2)k + 1) + (\Delta - 1)^2(1) + \Delta^2(k - 1) \\ &= (\Delta + 2)n - 3\Delta. \end{aligned}$$

Case 2. $2 \leq r < \Delta - 1$. As above, $n_2 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)r + (r - 1)$. Since $r - 1 < \Delta - 2$, it follows from Corollary 7 that

$(n_1, n_2, \dots, n_{r-1}, n_r, n_{r+1}, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k, 0, \dots, 0, 1, 0, \dots, 0, r, k - r)$ is the optimal solution. Since $2 \leq r < \Delta - 1$, it is easy to see that $2\Delta(1-r) + (r^2 + r - 2) < 0$ and we have

$$\begin{aligned} M_1(T) &= n_1 + 4n_2 + \dots + (\Delta - 2)^2 \cdot n_{\Delta-2} + (\Delta - 1)^2 \cdot n_{\Delta-1} + \Delta^2 \cdot n_{\Delta} \\ &= (\Delta - 2)k + r^2(1) + (\Delta - 1)^2 r + \Delta^2(k - r) \\ &= (\Delta + 2)(\Delta - 1)k + r^2 + r - 2r\Delta \\ &= (\Delta + 2)n - 3\Delta + 2\Delta(1 - r) + (r^2 + r - 2) \\ &< (\Delta + 2)n - 3\Delta. \end{aligned}$$

Case 3. $\Delta - 1 \leq r \leq k - 1$. There are non-negative integers t, s such that $r - 1 = t(\Delta - 2) + s$, $t \geq 1$ and $s < \Delta - 1$. By substituting in (4), we have $n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)(r + t) + s$. First let $0 < s$. Since $s \leq \Delta - 2$, it follows from Corollary 7 that

$(n_1, n_2, \dots, n_s, n_{s+1}, n_{s+2}, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k - t, 0, \dots, 0, 1, 0, \dots, 0, 0, r + t, k - r)$ is the optimal solution. Thus

$$\begin{aligned} M_1(T) &\leq (\Delta - 2)k - t + (s + 1)^2 + (\Delta - 1)^2(r + t) + \Delta^2(k - r) \\ &= (\Delta + 2)(\Delta - 1)k + (s + 1)^2 + r(1 - 2\Delta) + t\Delta(\Delta - 2) \\ &= (\Delta + 2)n - 3\Delta - s(\Delta - s - 2) - (r - 1)(\Delta - 1) \\ &< (\Delta + 2)n - 3\Delta. \end{aligned}$$

Now let $s = 0$. Then the optimal solution is

$(n_1, n_2, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k - t + 1, 0, \dots, 0, r + t, k - r)$ and we have

$$\begin{aligned} M_1(T) &\leq (\Delta - 2)k - t + 1 + (\Delta - 1)^2(r + t) + \Delta^2(k - r) \\ &= (\Delta + 2)(\Delta - 1)k - r(2\Delta - 1) + 1 + t\Delta(\Delta - 2) \\ &= (\Delta + 2)n - 3\Delta - (\Delta - 1)(r - 1) \\ &< (\Delta + 2)n - 3\Delta. \end{aligned}$$

As in the proof of Theorem 8 we can see that $M_1(T) = (\Delta + 2)n - 3\Delta$ if and only if $T \in \mathbb{T}_n$.

Theorem 10. Let T be a tree of order n with maximum degree Δ and $n \equiv p \pmod{\Delta - 1}$ where $2 \leq p \leq \Delta - 2$. Then

$$M_1(T) \leq \begin{cases} (\Delta + 2)n - 2\Delta - 2 & p = 2 \\ (\Delta + 2)n - 2\Delta - 3 + p(p - 2) & p \geq 3, \end{cases}$$

with equality if and only if $T \in \mathbb{T}_n$.

Proof. Let $n = (\Delta - 1)k + p$. Suppose that $r = \frac{n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} + (2 - p)}{\Delta - 1}$. By (4),

we have

$$n_{\Delta} = k - \left(\frac{n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} + (2 - p)}{\Delta - 1} \right) = k - r.$$

Then clearly $0 \leq r \leq k - 1$ and $1 \leq n_{\Delta} \leq k$. We consider four cases.

Case 1. $r = 0$. Then $n_{\Delta} = k$ and by (4) we have

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (n - 2) - ((\Delta - 1)n_{\Delta}) = ((\Delta - 1)k + p - 2) - (\Delta - 1)k = p - 2.$$

If $p = 2$, then $n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = 0$. This implies that $n_2 = n_3 = \dots = n_{\Delta-1} = 0$ and $n_1 = n - k$ by (2). Thus

$$\begin{aligned} M_1(T) &\leq n_1 + 2^2 n_2 + \dots + (\Delta - 1)^2 .n_{\Delta-1} + \Delta^2 .n_{\Delta} \\ &= (n - k) + \Delta^2 k \\ &= n + (\Delta + 1)(\Delta - 1)k \\ &= n + (\Delta + 1)(n - 2) \\ &= (\Delta + 2)n - 2\Delta - 2. \end{aligned}$$

Now let $2 < p \leq \Delta - 2$. Since $1 \leq p - 2 \leq \Delta - 4$ and $n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = p - 2$, it follows from Corollary 7 that

$$(n_1, n_2, \dots, n_{p-2}, n_{p-1}, n_p, \dots, n_{\Delta-1}, n_{\Delta}) = (n - k - 1, 0, \dots, 0, 1, 0, \dots, 0, k)$$

is the optimal solution and so

$$\begin{aligned} M_{1max}(T) &\leq n_1 + 4n_2 + \dots + (\Delta - 1)^2 .n_{\Delta-1} + \Delta^2 .n_{\Delta} \\ &= (n - k - 1) + (p - 1)^2 (1) + \Delta^2 (k) \\ &= (\Delta + 1)(\Delta - 1)k + n + p^2 - 2p \\ &= (\Delta + 1)(n - p) + n + p^2 - 2p \\ &= (\Delta + 2)n - p\Delta + p^2 - 3p. \end{aligned}$$

Case 2. $r = 1$. Then $n_{\Delta} = k - 1$ and

$$(n_1, n_2, \dots, n_{p-1}, n_p, n_{p+1}, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k + p - 1, 0, \dots, 0, 1, 0, \dots, 0, 1, k - 1)$$

is the optimal solution and since $p \leq \Delta - 2$ we have

$$\begin{aligned}
 M_1(T) &= n_1 + 4n_2 + \dots + (\Delta - 1)^2 . n_{\Delta-1} + \Delta^2 . n_{\Delta} \\
 &= (\Delta - 2)k + p - 1 + p^2 + (\Delta - 1)^2 + \Delta^2(k - 1) \\
 &= \Delta k - 2k + p - 1 + p^2 + \Delta^2 - 2\Delta + 1 + \Delta^2 k - \Delta^2 \\
 &= (\Delta + 2)(\Delta - 1)k + p + p^2 - 2\Delta \\
 &= (\Delta + 2)(n - p) + p + p^2 - 2\Delta \\
 &< (\Delta + 2)n - p\Delta + p^2 - 3p.
 \end{aligned}$$

Case 3. $2 \leq r < \Delta - p$. By (4), we have $n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)r + (p + r - 2)$. Since $r - 2 < \Delta - 2$, it follows from Corollary 7 that $(n_1, n_2, \dots, n_{p+r-2}, n_{p+r-1}, n_{p+r}, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k + p - 1, 0, \dots, 0, 1, 0, \dots, 0, r, k - r)$ is the optimal solution. On the other hand, we deduce from $p \leq \Delta - 2$ and $r < \Delta - p$ that $r - 1 + 2(p - \Delta) < \Delta - p - 1 + 2(p - \Delta) = p - \Delta - 1 < 0$ and so $r(r - 1 + 2(p - \Delta)) < 0$. Thus

$$\begin{aligned}
 M_1(T) &\leq n_1 + 4n_2 + \dots + (\Delta - 1)^2 . n_{\Delta-1} + \Delta^2 . n_{\Delta} \\
 &= ((\Delta - 2)k + p - 1) + (p + r - 1)^2(1) + (\Delta - 1)^2(r) + \Delta^2(k - r) \\
 &= \Delta k - 2k + p - 1 + p^2 + r^2 + 1 + 2rp - 2p - 2r + r\Delta^2 - 2\Delta r + r + \Delta^2 k - r\Delta^2 \\
 &= (\Delta + 2)(\Delta - 1)k + p^2 - p - 2\Delta r + r(r + 2p - 1) \\
 &= (\Delta + 2)(n - p) + p^2 - p - 2\Delta r + r(r + 2p - 1) \\
 &= (\Delta + 2)n - p\Delta + p^2 - 3p + r(r - 1 + 2(p - \Delta)) \\
 &< (\Delta + 2)n - p\Delta + p^2 - 3p = M_{1max}(T).
 \end{aligned}$$

Case 4. $\Delta - p \leq r \leq k - 1$. Let $p + r - 2 = t(\Delta - 2) + s$. By substituting in (4), we have $n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)(r + t) + s$. If $s = 0$ then by Corollary 7,

$(n_1, n_2, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k + p - t, 0, \dots, 0, r + t, k - r)$ is the optimal solution. Since $\Delta - p \leq r$ and $p \leq \Delta - 2$, we have

$$\begin{aligned}
 (2p - p^2 + p\Delta - \Delta r - 2\Delta + r) &= p(\Delta - p + 2) - \Delta r - 2\Delta + r \\
 &\leq p(r + 2) - \Delta r - 2\Delta + r \\
 &= (p - \Delta)(r + 2) + r \\
 &< (p - \Delta)(r + 2) + (r + 2) \\
 &= (p - \Delta + 1)(r + 2) < 0.
 \end{aligned}$$

Thus

$$\begin{aligned}
 M_1(T) &= n_1 + 4n_2 + \dots + (\Delta - 1)^2 \cdot n_{\Delta-1} + \Delta^2 \cdot n_{\Delta} \\
 &= ((\Delta - 2)k + p - t) + (\Delta - 1)^2(r + t) + \Delta^2(k - r) \\
 &= (\Delta^2k + \Delta k - 2k) + \Delta t(\Delta - 2) + p - 2\Delta r + r \\
 &= (\Delta + 2)(n - p) + \Delta t(\Delta - 2) + p - 2\Delta r + r \\
 &= (\Delta + 2)n - p\Delta - 2p + p\Delta + \Delta r + p - 2\Delta - 2\Delta r + r \\
 &= (\Delta + 2)n - p\Delta + p^2 - 3p + (2p - p^2 + p\Delta - \Delta r - 2\Delta + r) \\
 &< (\Delta + 2)n - p\Delta + p^2 - 3p.
 \end{aligned}$$

Now let $0 < s$. Since $s < \Delta - 2$, it follows from Corollary 7 that $(n_1, n_2, \dots, n_s, n_{s+1}, n_{s+2}, \dots, n_{\Delta-2}, n_{\Delta-1}, n_{\Delta}) = ((\Delta - 2)k + p - (t + 1), 0, \dots, 0, 1, 0, \dots, 0, 0, r + t, k - r)$ is the optimal solution. Since $2 \leq p \leq \Delta - 2$ and $0 < s \leq \Delta - 3$, it is straightforward to verify that $p\Delta - p^2 + 2p + s^2 + 2s - \Delta r + r - 2\Delta - \Delta s < 0$. Thus

$$\begin{aligned}
 M_1(T) &= n_1 + 4n_2 + \dots + (\Delta - 1)^2 \cdot n_{\Delta-1} + \Delta^2 \cdot n_{\Delta} \\
 &= (\Delta - 2)k + p - (t + 1) + (s + 1)^2 + (\Delta - 1)^2(r + t) + \Delta^2(k - r) \\
 &= (\Delta^2k + \Delta k - 2k) + p + s^2 + 2s - 2\Delta r + r + \Delta^2t - 2\Delta t \\
 &= (\Delta + 2)(\Delta - 1)k + p + s^2 + 2s - 2\Delta r + r + \Delta t(\Delta - 2) \\
 &= (\Delta + 2)(n - p) + p + s^2 + 2s - 2\Delta r + r + \Delta(p + r - 2 - s) \\
 &= (\Delta + 2)n - p + s^2 + 2s - \Delta r + r - 2\Delta - \Delta s \\
 &= (\Delta + 2)n - p\Delta + p^2 - 3p + (p\Delta - p^2 + 2p + s^2 + 2s - \Delta r + r - 2\Delta - \Delta s) \\
 &< (\Delta + 2)n - p\Delta + p^2 - 3p.
 \end{aligned}$$

Therefore, in all cases $M_1(T) \leq (\Delta + 2)n - p\Delta + p^2 - 3p$. As in the proof of Theorem 8, we can see that

$$M_1(T) = \begin{cases} (\Delta + 2)n - 2\Delta - 2 & p = 2 \\ (\Delta + 2)n - 2\Delta - 3 + p(p - 2) & p \geq 3, \end{cases}$$

if and only if $T \in \mathbb{T}_n$. This completes the proof.

We now present a lower bound on the first Zagreb coindex among all trees. Ashrafi et al. [1] proved that for any conneted graph G of order n and size m

$$\overline{M}_1(G) = 2m(n - 1) - M_1(G).$$

Next result is an immediate consequence of this equality and Theorem 1.

Corollary 11. Let T be a tree of order n with maximum degree Δ . If $n \equiv p \pmod{\Delta-1}$, then

$$\overline{M}_1(T) \leq \begin{cases} -(\Delta+6)n + 2n^2 + 4\Delta - 2 & p = 0 \\ -(\Delta+6)n + 2n^2 + 3\Delta + 2 & p = 1 \\ -(\Delta+6)n + 2n^2 + 2\Delta + 4 & p = 2. \\ -(\Delta+6)n + 2n^2 + p\Delta + 2 - p(p-3) & p \geq 3. \end{cases}$$

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An upper bound on the first Zagreb index in trees

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کران بالای شاخص زاگرب اول در درختها

ادیتور رابطا : علیرضا اشرفی

چکیده

شاخص زاگرب اول برابر مجموع مربعات درجات راس‌های گراف می‌باشد و با $M_1(G)$ نمایش داده می‌شود و هم‌اندیس اول گراف برابر مجموع درجات زوج راس‌های غیرمجاور است. ووکیسویچ و پاپیوودا در مرجع [Iran. J. Math. Chem. 5 (2014) 19-29] ثابت کردند که برای هر درخت شیمیایی از مرتبه n ، $n \geq 5$ ،

$$M_1(T) \leq \begin{cases} 6n-12 & n \equiv 0,1 \pmod{3} \\ 6n-10 & \text{otherwise.} \end{cases}$$

در این مقاله کران بالای اندیس زاگرب اول در همه درختها بر حسب تعداد راس‌ها و ماکزیمم درجه، تعمیم یافته است. همچنین کران پایین برای هم‌اندیس زاگرب اول درختها محاسبه شده است.

لغات کلیدی: اندیس زاگرب اول، هم‌اندیس زاگرب اول، درخت، درخت شیمیایی