



Zeroth-order General Randić Index of Trees

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ABSTRACT: Randić indices belong to the most well-known topological indices. We study a very general index called the zeroth-order general Randić index. We present upper and lower bounds on the zeroth-order general Randić index for trees with given order and independence number, and for trees with given order and domination number. We also show that the bounds are best possible.

Key Words: Zeroth-order general Randić index, Tree, Independence number, Domination number.

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1. Introduction

Topological indices have been studied because of their extensive applications. These indices are graph invariants that play a significant role in chemistry, materials science, pharmaceutical sciences and engineering, since they can be correlated with a large number of physico-chemical properties of molecules. Randić indices belong to the most well-known topological indices. We use graph theory to study the zeroth-order general Randić index.

Let G be a graph with the vertex set $V(G)$ and the edge set $E(G)$. The order n of a graph G is the number of vertices of G . The degree of a vertex $v \in V(G)$ is the number of edges incident with v and it is denoted by $d_G(v)$ (or simply $d(v)$). We denote the star and the path graph of order n by S_n and P_n , respectively. A tree T is a graph containing no cycles. A leaf is a vertex of T having degree one.

An independent set S is a subset of $V(G)$ such that no two vertices in S are adjacent. The independence number $\alpha(G)$ is the number of vertices in a maximum independent set of G . A dominating set D is a subset of $V(G)$ such that every vertex not in D is adjacent to at least one vertex in D . The domination number $\gamma(G)$ of a graph G is the cardinality of a smallest dominating set.

The zeroth-order general Randić index of a graph G is defined as

$$M_1^a(G) = \sum_{v \in V(G)} d_G(v)^a$$

where $a \neq 0$ is a real number. If $a = 2$, we obtain the well-known first Zagreb index $M_1(G) = \sum_{v \in V(G)} d_G(v)^2$.

Khalid and Ali [7] studied trees of given order and given number of leaves/segments/branching vertices and they determined the maximum and minimum zeroth-order general Randić index for those trees. Yamaguchi [12] obtained the largest zeroth-order general Randić index for trees of given order, and given diameter or radius. An upper bound on the zeroth-order general Randić index for trees of given order and independence number, where $a > 1$, was presented by Tomescu and Jamil [9].

Bounds on Zagreb indices for trees with given order and domination number were given by Borovičanin and Furtula [2] and trees with given independence number were studied in [3] and [10]. Kazemi and Behtoei [6] obtained the mean value of the first Zagreb index for d -ary trees. Lin [8] characterized trees

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which minimize and maximize the first Zagreb index among all trees with fixed number of segments. Upper and lower bounds on the first Zagreb index of apex trees were presented in [1]. Various Zagreb indices for trees were studied in numerous papers, see for example [4], [5] and [11].

We present bounds on the zeroth-order general Randić index for trees with given order and independence number, and for trees with given order and domination number. We also show that the bounds are sharp.

2. Preliminary results

We use Lemma 2.2 in the proof of Theorem 3.1 and Lemma 2.1 in the proofs of Theorems 3.2 and 3.3. Lemmas 2.1 and 2.2 can be stated in a more general form. We keep them simple, because this form is sufficient for us and it is easy to follow the proofs.

Lemma 2.1. *Let $1 \leq x_1 \leq x_2$. For $a > 1$ and $a < 0$, we have*

$$(x_1 + 1)^a - x_1^a \leq (x_2 + 1)^a - x_2^a.$$

If $0 < a < 1$, then

$$(x_1 + 1)^a - x_1^a \geq (x_2 + 1)^a - x_2^a.$$

Equalities hold if and only if $x_1 = x_2$.

Proof. Let us study the function

$$f(x) = (x + 1)^a - x^a.$$

for $x \geq 1$. The derivative

$$f'(x) = a[(x + 1)^{a-1} - x^{a-1}].$$

If $a > 1$, then $(x + 1)^{a-1} > x^{a-1}$, thus $f'(x) > 0$ which means that $f(x)$ is a strictly increasing function.

Let $a < 1$. Then $1 - a = c > 0$. We have

$$(x + 1)^{a-1} - x^{a-1} = \left(\frac{1}{x+1}\right)^c - \left(\frac{1}{x}\right)^c < 0$$

since $0 < \frac{1}{x+1} < \frac{1}{x} \leq 1$ which means that $\left(\frac{1}{x+1}\right)^c < \left(\frac{1}{x}\right)^c$. Thus if $a < 0$, then $f'(x) > 0$, so $f(x)$ is a strictly increasing function. If $0 < a < 1$, then $f'(x) < 0$ and $f(x)$ is a strictly decreasing function.

Hence for $a > 1$ and $a < 0$, if $x_1 \leq x_2$, then $f(x_1) \leq f(x_2)$ which gives

$$(x_1 + 1)^a - x_1^a \leq (x_2 + 1)^a - x_2^a.$$

For $0 < a < 1$, if $x_1 \leq x_2$, then $f(x_1) \geq f(x_2)$ which gives

$$(x_1 + 1)^a - x_1^a \geq (x_2 + 1)^a - x_2^a.$$

Clearly, equalities hold if and only if $x_1 = x_2$. □

Lemma 2.2. *Let $2 \leq x_1 \leq x_2$. For $a > 1$ and $a < 0$, we have*

$$x_1^a + x_2^a < (x_1 - 1)^a + (x_2 + 1)^a.$$

If $0 < a < 1$, then

$$x_1^a + x_2^a > (x_1 - 1)^a + (x_2 + 1)^a.$$

Proof. Let $x \geq 1$. From the proof of Lemma 2.2 we know that the function

$$f(x) = (x + 1)^a - x^a$$

is strictly increasing for $a > 1$ and $a < 0$. So if $2 \leq x_1 \leq x_2$, then $f(x_1 - 1) < f(x_2)$ which gives

$$x_1^a + x_2^a < (x_1 - 1)^a + (x_2 + 1)^a.$$

For $0 < a < 1$, $f(x)$ is strictly decreasing. Thus if $2 \leq x_1 \leq x_2$, then $f(x_1 - 1) > f(x_2)$ which gives

$$x_1^a + x_2^a > (x_1 - 1)^a + (x_2 + 1)^a.$$

□

3. Main results

Any tree with n vertices is a bipartite graph and each partite set is an independent set. One of the partite sets has at least $\frac{n}{2}$ vertices, thus for every tree T we obtain $\alpha(T) \geq \frac{n}{2}$. Note that $\alpha(T) \leq n - 1$ and the equality holds for stars. Therefore for any tree having n vertices and independence number s , we get $\frac{n}{2} \leq s \leq n - 1$.

In Theorems 3.1 and 3.2 we present upper and lower bounds on the zeroth-order general Randić index for trees of given order and independence number.

Theorem 3.1. *Let T be a tree having order n and independence number s . For $a > 1$ and $a < 0$, we have*

$$M_1^a(T) \geq (n - 1 - (n - s)p)(p + 1)^a + (1 - s + (n - s)p)p^a + (n - s - 1)2^a + 2s - n + 1,$$

and if $0 < a < 1$, then

$$M_1^a(T) \leq (n - 1 - (n - s)p)(p + 1)^a + (1 - s + (n - s)p)p^a + (n - s - 1)2^a + 2s - n + 1,$$

where $p = \left\lfloor \frac{n-1}{n-s} \right\rfloor$. The bounds are sharp.

Proof. Let T be a tree of order n having independence number s . Let S be any independent set in T having s vertices. We define $\bar{S} = V(T) \setminus S$. Note that $|\bar{S}| = n - s$. Let y be the number of edges uv with $u \in S$ and $v \in \bar{S}$. We denote by z the number of edges between vertices in \bar{S} . The set S is an independent set, thus there are no edges between vertices of S . Every tree has $n - 1$ edges, so we obtain $z + y = n - 1$. We have

$$\sum_{u \in S} d(u) = y = n - z - 1$$

and

$$\sum_{u \in S} d(u) + \sum_{u \in \bar{S}} d(u) = \sum_{u \in V(T)} d(u) = 2|E(T)| = 2n - 2,$$

thus

$$\sum_{u \in \bar{S}} d(u) = \sum_{u \in V(T)} d(u) - \sum_{u \in S} d(u) = n + z - 1.$$

We know that

$$M_1^a(T) = \left(\sum_{u \in S} d(u)^a \right) + \left(\sum_{u \in \bar{S}} d(u)^a \right).$$

By Lemma 2.2, the sum $\sum_{u \in S} d(u)^a$ is smallest for $a > 1$ and $a < 0$ (the sum $\sum_{u \in S} d(u)^a$ is largest for $0 < a < 1$) if $d(u)$ and $d(v)$ differ by at most one for any $u, v \in S$. We have $|S| = s$, thus $d(u), d(v) \in \left\{ \left\lfloor \frac{y}{s} \right\rfloor, \left\lceil \frac{y}{s} \right\rceil \right\}$. Similarly, $\sum_{u \in \bar{S}} d(u)^a$ is smallest for $a > 1$ and $a < 0$ ($\sum_{u \in \bar{S}} d(u)^a$ is largest for $0 < a < 1$) if $d(u)$ and $d(v)$ differ by at most one for any $u, v \in \bar{S}$. We have $|\bar{S}| = n - s$, thus $d(u), d(v) \in \left\{ \left\lfloor \frac{n+z-1}{n-s} \right\rfloor, \left\lceil \frac{n+z-1}{n-s} \right\rceil \right\}$.

Since $d(u) \geq 1$, we obtain $\sum_{u \in S} d(u) \geq s$, thus $y \geq s$ and $1 \leq \frac{y}{s}$. We know that for trees $s \geq \frac{n}{2}$, therefore

$$1 \leq \frac{y}{s} = \frac{n - z - 1}{s} \leq \frac{n - 1}{\frac{n}{2}} < 2.$$

Thus $\left\lfloor \frac{y}{s} \right\rfloor = 1$ which means that $y = s + t$ where $0 \leq t < s$. So $\sum_{u \in S} d(u)^a$ is smallest for $a > 1$ and $a < 0$ ($\sum_{u \in S} d(u)^a$ is largest for $0 < a < 1$) if S contains t vertices having degree 2 and $s - t$ vertices having degree 1. Then for $a > 1$ and $a < 0$,

$$\begin{aligned} \sum_{u \in S} d(u)^a &\geq t2^a + (s - t)1^a = (y - s)2^a + (s - (y - s)) = (y - s)2^a + 2s - y \\ &= (n - z - 1 - s)2^a + 2s - n + z + 1. \end{aligned}$$

If $0 < a < 1$, then

$$\sum_{u \in \overline{S}} d(u)^a \leq (n - z - 1 - s)2^a - n + z + 1.$$

We have $\sum_{u \in \overline{S}} d(u) = n + z - 1$ and $|\overline{S}| = n - s$, therefore $n + z - 1 \geq n - s$. Let $n + z - 1 = (n - s)k + l$ where $k = \left\lfloor \frac{n+z-1}{n-s} \right\rfloor$ and $0 \leq l < n - s$. Then $l = n + z - 1 - (n - s) \left\lfloor \frac{n+z-1}{n-s} \right\rfloor$. The sum $\sum_{u \in \overline{S}} d(u)^a$ is smallest for $a > 1$ and $a < 0$ ($\sum_{u \in \overline{S}} d(u)^a$ is largest for $0 < a < 1$) if \overline{S} contains l vertices having degree $k + 1$ and $n - s - l$ vertices having degree k . Let us use k instead of $\left\lfloor \frac{n+z-1}{n-s} \right\rfloor$ in the next paragraphs. For $a > 1$ and $a < 0$, we get

$$\begin{aligned} \sum_{u \in \overline{S}} d(u)^a &\geq l(k+1)^a + (n-s-l)k^a \\ &= (n+z-1-(n-s)k)(k+1)^a + (n-s-(n+z-1-(n-s)k))k^a \\ &= (n+z-1-(n-s)k)(k+1)^a + (1-s-z+(n-s)k)k^a \end{aligned}$$

and

$$\begin{aligned} M_1^a(T) &\geq (n-z-1-s)2^a + 2s - n + z + 1 \\ &\quad + (n+z-1-(n-s)k)(k+1)^a + (1-s-z+(n-s)k)k^a = f(z). \end{aligned}$$

For $0 < a < 1$,

$$\sum_{u \in \overline{S}} d(u)^a \leq (n+z-1-(n-s)k)(k+1)^a + (1-s-z+(n-s)k)k^a$$

and

$$\begin{aligned} M_1^a(T) &\leq (n-z-1-s)2^a + 2s - n + z + 1 \\ &\quad + (n+z-1-(n-s)k)(k+1)^a + (1-s-z+(n-s)k)k^a = f(z). \end{aligned}$$

We have $s \leq y = n - z - 1$, thus $0 \leq z \leq n - 1 - s$ and

$$\frac{n-1}{n-s} \leq \frac{n+z-1}{n-s} \leq \frac{n-2}{n-s} + 1 < \frac{n-1}{n-s} + 1.$$

This means that the interval $\left[\frac{n-1}{n-s}, \frac{n-1}{n-s} + 1 \right)$ contains exactly one integer. If $z = (n-s) \left\lfloor \frac{n-1}{n-s} \right\rfloor - s + 1$, we get $\frac{n+z-1}{n-s} = \left\lfloor \frac{n-1}{n-s} \right\rfloor + 1$. This means that

$$k = \left\lfloor \frac{n-1}{n-s} \right\rfloor \quad \text{for } 0 \leq z < (n-s) \left\lfloor \frac{n-1}{n-s} \right\rfloor - s + 1 \quad (3.1)$$

and

$$k = \left\lfloor \frac{n-1}{n-s} \right\rfloor + 1 \quad \text{for } (n-s) \left\lfloor \frac{n-1}{n-s} \right\rfloor - s + 1 \leq z \leq n - s - 1. \quad (3.2)$$

Then

$$\begin{aligned} f(z) &= z((k+1)^a + 1 - k^a - 2^a) + (n-1-(n-s)k)(k+1)^a \\ &\quad + (1-s+(n-s)k)k^a + (n-1-s)2^a + 2s - n + 1. \end{aligned}$$

We show that Theorem 3.1 holds for $k = 1$. Note that $z \geq 0$ and $s \geq \left\lfloor \frac{n}{2} \right\rfloor$. Thus

$$\frac{n+z-1}{n-s} \geq \frac{n-1}{\left\lfloor \frac{n}{2} \right\rfloor} = \begin{cases} 2 & \text{if } n \text{ is odd,} \\ 2 - \frac{2}{n} & \text{if } n \text{ is even.} \end{cases}$$

So $k = 1$ if and only if n is even, $z = 0$ and $s = \frac{n}{2}$. This is satisfied only by paths with $2s$ vertices if $d(u)$ and $d(v)$ differ by at most one for $u, v \in S$ and $u, v \in \bar{S}$. Note that paths satisfy the bound given in Theorem 3.1.

So let us suppose that $k \geq 2$. By Lemma 2.2, for $a > 1$ and $a < 0$, we have $(k+1)^a + 1 - k^a - 2^a > 0$, thus $z_1((k+1)^a + 1 - k^a - 2^a) < z_2((k+1)^a + 1 - k^a - 2^a)$ for $z_1 < z_2$. Therefore if z is in the interval obtained in (3.1), $f(z)$ is smallest for $z = 0$. If z is in the interval obtained in (3.2), $f(z)$ is smallest for $z' = (n-s) \left\lfloor \frac{n-1}{n-s} \right\rfloor - s + 1$.

If $0 < a < 1$, then $(k+1)^a + 1 - k^a - 2^a < 0$, thus $z_1((k+1)^a + 1 - k^a - 2^a) > z_2((k+1)^a + 1 - k^a - 2^a)$ for $z_1 < z_2$. Therefore if z is in the interval obtained in (3.1), $f(z)$ is largest for $z = 0$. If z is in the interval obtained in (3.2), $f(z)$ is largest for $z' = (n-s) \left\lfloor \frac{n-1}{n-s} \right\rfloor - s + 1$.

We compare $f(0)$ and $f(z')$. Let $p = \left\lfloor \frac{n-1}{n-s} \right\rfloor$. We get $k = p$ for $z = 0$ and $k = p+1$ for $z' = (n-s)p - s + 1$. We obtain

$$\begin{aligned} f(z') &= z'((p+2)^a + 1 - (p+1)^a - 2^a) \\ &\quad - z'(p+2)^a + (z' + n - s)(p+1)^a + (n-1-s)2^a + 2s - n + 1 \\ &= z'(1 - 2^a) + (n-s)(p+1)^a + (n-1-s)2^a + 2s - n + 1 \end{aligned}$$

and

$$f(0) = (n-1 - (n-s)p)(p+1)^a + (1-s + (n-s)p)p^a + (n-1-s)2^a + 2s - n + 1.$$

Consequently, for $a > 1$ and $a < 0$,

$$f(z') - f(0) = z'((p+1)^a + 1 - p^a - 2^a) > 0$$

for $p \geq 2$ since from Lemma 2.2 we have $(p+1)^a + 1 - p^a - 2^a > 0$. Therefore $f(z') > f(0)$ which yields $M_1^a(T) \geq f(0)$.

If $0 < a < 1$, then

$$f(z') - f(0) = z'((p+1)^a + 1 - p^a - 2^a) < 0$$

for $p \geq 2$ since from Lemma 2.2 we have $(p+1)^a + 1 - p^a - 2^a < 0$. Therefore $f(z') < f(0)$ which yields $M_1^a(T) \leq f(0)$.

If $p = \left\lfloor \frac{n-1}{n-s} \right\rfloor = 1$, we get $s = \frac{n}{2}$. Otherwise if $s \geq \frac{n+1}{2}$, we would obtain $\left\lfloor \frac{n-1}{n-s} \right\rfloor \geq 2$. So $s = \frac{n}{2}$ and it holds only for paths if $d(u)$ and $d(v)$ differ by at most one for $u, v \in S$ and $u, v \in \bar{S}$. Note that paths satisfy the bound stated in Theorem 3.1.

We show that the bounds are sharp. Let T be a tree with $z = 0$, which implies that \bar{S} is also an independent set, where degrees of any two vertices in S differ by at most one and degrees of any two vertices in \bar{S} differ by at most one. Then

$$M_1^a(T) = f(0) = (n-1 - (n-s)p)(p+1)^a + (1-s + (n-s)p)p^a + (n-1-s)2^a + 2s - n + 1$$

where $p = \left\lfloor \frac{n-1}{n-s} \right\rfloor$. Hence the bounds stated in Theorem 3.1 are sharp. \square

Theorem 3.2. *Let T be a tree having order n and independence number s . Then for $a > 1$ and $a < 0$,*

$$M_1^a(T) \leq s^\alpha + s + 2^\alpha(n-s-1).$$

If $0 < a < 1$, then

$$M_1^a(T) \geq s^\alpha + s + 2^\alpha(n-s-1).$$

The bounds are sharp.

Proof. The bound holds for small n . For $n = 2$, the only tree is the path P_2 and we have $s = 1$. If $n = 3$, we get P_3 and $s = 2$. For $n = 4$ we have two trees, namely S_4 if $s = 3$ and P_4 if $s = 2$, and the bound is again satisfied.

Let us prove Theorem 3.2 by induction on n . Let T be a tree with n vertices and independence number s , where $n \geq 5$ and $\frac{n}{2} < s < n - 1$ (cases $s = \frac{n}{2}$ and $s = n - 1$ are discussed at the end of this proof). Assume that the bound is satisfied for trees having $n' = n - 1$ vertices (their independence number is $s' = s$ or $s' = s - 1$). This means that for $\frac{n}{2} < s < n - 1$, we have $\frac{n'}{2} \leq s' \leq n' - 1$.

Let $v_1 v_2 \dots v_{d+1}$ be any path having length d in T , where d is the diameter of T . So v_1 and v_{d+1} are leaves. Let $d_T(v_2) = k$. We obtain $k \leq s$. Let S be any maximum independent set of T . Let T_1 be a tree with $V(T_1) = V(T) \setminus \{v_1\}$ and $E(T_1) = E(T) \setminus \{v_1 v_2\}$. Let us consider two cases.

Case 1: $v_1 \notin S$.

Then $\alpha(T_1) = s$. If v_2 would be adjacent to $w \notin \{v_1, v_3\}$ in T that is not a leaf, we get a path of length at least $d + 1$ in T . If v_2 would be adjacent to $w \notin \{v_1, v_3\}$ that is a leaf, then v_1 and w must be in every maximum independent set (which means that $v_1 \in S$). Thus v_1 and v_3 are the only neighbours of v_2 in T . Therefore $d_T(v_1) = 1$, $d_T(v_2) = 2$, $d_{T_1}(v_2) = 1$ and

$$M_1^a(T) - M_1^a(T_1) = 2^\alpha.$$

Since T_1 has order $n - 1$ and independence number s , for $a > 1$ and $a < 0$, by the induction hypothesis we get

$$M_1^a(T_1) \leq s^\alpha + s + 2^\alpha((n - 1) - s - 1).$$

Then

$$M_1^a(T) = M_1^a(T_1) + 2^\alpha \leq s^\alpha + s + 2^\alpha(n - s - 1).$$

If $0 < a < 1$, then by the induction hypothesis we get

$$M_1^a(T_1) \geq s^\alpha + s + 2^\alpha((n - 1) - s - 1).$$

Thus

$$M_1^a(T) = M_1^a(T_1) + 2^\alpha \geq s^\alpha + s + 2^\alpha(n - s - 1).$$

Case 2: $v_1 \in S$.

Then $\alpha(T_1) = s - 1$. We have $d_T(v_1) = 1$, $d_T(v_2) = k$ and $d_{T_1}(v_2) = k - 1$, thus

$$M_1^a(T) - M_1^a(T_1) = 1 + k^\alpha - (k - 1)^\alpha.$$

Note that T_1 has order $n - 1$ and independence number $s - 1$, so for $a > 1$ and $a < 0$, by the induction hypothesis we get

$$M_1^a(T_1) \leq (s - 1)^\alpha + (s - 1) + 2^\alpha((n - 1) - (s - 1) - 1).$$

Thus

$$M_1^a(T) = M_1^a(T_1) + 1 + k^\alpha - (k - 1)^\alpha \leq (s - 1)^\alpha + (s - 1) + 2^\alpha(n - s - 1) + 1 + k^\alpha - (k - 1)^\alpha.$$

Since by Lemma 2.1, $k^\alpha - (k - 1)^\alpha \leq s^\alpha - (s - 1)^\alpha$, we get

$$M_1^a(T) \leq s^\alpha + s + 2^\alpha(n - s - 1).$$

If $0 < a < 1$, then by the induction hypothesis we get

$$M_1^a(T_1) \geq (s - 1)^\alpha + (s - 1) + 2^\alpha((n - 1) - (s - 1) - 1).$$

Thus

$$M_1^a(T) \geq (s - 1)^\alpha + (s - 1) + 2^\alpha(n - s - 1) + 1 + k^\alpha - (k - 1)^\alpha.$$

Since by Lemma 2.1, $k^\alpha - (k - 1)^\alpha \geq s^\alpha - (s - 1)^\alpha$, we get

$$M_1^a(T) \geq s^\alpha + s + 2^\alpha(n - s - 1).$$

It is easy to check that the bound is satisfied if $s = \frac{n}{2}$ and if $s = n - 1$. If $s = n - 1$, we obtain a star and for stars S_n we get $M_1^a(S_n) = (n - 1)^\alpha + n - 1$. If $s = \frac{n}{2}$, then both partite sets of T (which is a bipartite graph) have $\frac{n}{2}$ vertices. Each partite set is an independent set of T , so there is an independent set not containing the leaf v_1 . Then we can use Case 1 and prove the bound by induction.

Let us show that the bounds are sharp. Let T be a tree containing one vertex w having degree s , where w is adjacent to $2s - n + 1$ leaves and $n - s - 1$ vertices of degree 2 such that every vertex of degree 2 is adjacent to a leaf. The vertices adjacent to w form a maximum independent set. The order of T is n and the independence number is s . We have

$$M_1^a(T) = s^\alpha + s + 2^\alpha(n - s - 1),$$

therefore the bounds are sharp. \square

Any tree of order n is a bipartite graph and each partite set is a dominating set. One of the partite sets has at most $\frac{n}{2}$ vertices, thus for every tree T we obtain $\gamma(T) \leq \frac{n}{2}$. Note that $\gamma(S_n) = 1$. Therefore for any tree having n vertices and dominating number γ , we get $1 \leq \gamma \leq \frac{n}{2}$.

Let us state bounds on the zeroth-order general Randić index for trees of given order and domination number.

Theorem 3.3. *Let T be a tree having order n and domination number γ . Then for $a > 1$ and $a < 0$,*

$$M_1^a(T) \leq (n - \gamma)^\alpha + n - \gamma + 2^\alpha(\gamma - 1).$$

If $0 < a < 1$, then

$$M_1^a(T) \geq (n - \gamma)^\alpha + n - \gamma + 2^\alpha(\gamma - 1).$$

The bounds are sharp.

Proof. The bound holds for small n . For $n = 2$, the only tree is the path P_2 . If $n = 3$, we get P_3 . In both cases $\gamma = 1$. For $n = 4$ we have two trees, namely S_4 if $\gamma = 1$ and P_4 if $\gamma = 2$, and the bound is again satisfied.

Let us prove Theorem 3.3 by induction on n . Let T be a tree with n vertices and domination number γ , where $n \geq 5$ and $1 < \gamma < \frac{n}{2}$ (cases $\gamma = 1$ and $\gamma = \frac{n}{2}$ are discussed at the end of this proof). Assume that the bound is satisfied for trees having $n' = n - 1$ vertices (their domination number is $\gamma' = \gamma$ or $\gamma' = \gamma - 1$). This means that for $1 < \gamma < \frac{n}{2}$, we have $1 \leq \gamma' \leq \frac{n'}{2}$.

Let $v_1 v_2 \dots v_{d+1}$ be any path having length d in T , where d is the diameter of T . So v_1 and v_{d+1} are leaves. Let $d_T(v_2) = k$. Clearly, all vertices except for the neighbours of v_2 also form a dominating set of T , which means that $\gamma \leq n - k$. Thus $k \leq n - \gamma$. Let D be any smallest dominating set of T . Let T_1 be a tree with $V(T_1) = V(T) \setminus \{v_1\}$ and $E(T_1) = E(T) \setminus \{v_1 v_2\}$. Let us consider two cases.

Case 1: $v_1 \notin D$.

Then $\gamma(T_1) = \gamma$. We have $d_T(v_1) = 1$, $d_T(v_2) = k$ and $d_{T_1}(v_2) = k - 1$, thus

$$M_1^a(T) - M_1^a(T_1) = 1 + k^\alpha - (k - 1)^\alpha.$$

Note that T_1 has order $n - 1$ and domination number γ , so for $a > 1$ and $a < 0$, by the induction hypothesis we get

$$M_1^a(T_1) \leq ((n - 1) - \gamma)^\alpha + (n - 1) - \gamma + 2^\alpha(\gamma - 1).$$

Thus

$$M_1^a(T) = M_1^a(T_1) + 1 + k^\alpha - (k - 1)^\alpha \leq (n - \gamma - 1)^\alpha + n - \gamma - 1 + 2^\alpha(\gamma - 1) + 1 + k^\alpha - (k - 1)^\alpha.$$

Since by Lemma 2.1, $k^\alpha - (k - 1)^\alpha \leq (n - \gamma)^\alpha - (n - \gamma - 1)^\alpha$, we get

$$M_1^a(T) \leq (n - \gamma)^\alpha + n - \gamma + 2^\alpha(\gamma - 1).$$

If $0 < a < 1$, then by the induction hypothesis we get

$$M_1^a(T_1) \geq ((n-1) - \gamma)^\alpha + (n-1) - \gamma + 2^\alpha(\gamma-1).$$

Thus

$$M_1^a(T) \geq (n - \gamma - 1)^\alpha + n - \gamma - 1 + 2^\alpha(\gamma - 1) + 1 + k^\alpha - (k - 1)^\alpha.$$

Since by Lemma 2.1, $k^\alpha - (k - 1)^\alpha \geq (n - \gamma)^\alpha - (n - \gamma - 1)^\alpha$, we get

$$M_1^a(T) \geq (n - \gamma)^\alpha + n - \gamma + 2^\alpha(\gamma - 1).$$

Case 2: $v_1 \in D$.

Then $\gamma(T_1) = \gamma - 1$. If v_2 would be adjacent to $w \notin \{v_1, v_3\}$ in T that is not a leaf, we get a path of length at least $d + 1$ in T . If v_2 would be adjacent to $w \notin \{v_1, v_3\}$ that is a leaf, then v_2 must be in every smallest dominating set (which means that $v_1 \notin D$). Thus v_1 and v_3 are the only neighbours of v_2 in T . So $d_T(v_1) = 1$, $d_T(v_2) = 2$, $d_{T_1}(v_2) = 1$ and

$$M_1^a(T) - M_1^a(T_1) = 2^\alpha.$$

Since T_1 has order $n - 1$ and domination number $\gamma - 1$, for $a > 1$ and $a < 0$, by the induction hypothesis we get

$$M_1^a(T_1) \leq ((n-1) - (\gamma-1))^\alpha + (n-1) - (\gamma-1) + 2^\alpha((\gamma-1) - 1).$$

Then

$$M_1^a(T) = M_1^a(T_1) + 2^\alpha \leq (n - \gamma)^\alpha + n - \gamma + 2^\alpha(\gamma - 2) + 2^\alpha.$$

If $0 < a < 1$, then by the induction hypothesis we get

$$M_1^a(T_1) \geq ((n-1) - (\gamma-1))^\alpha + (n-1) - (\gamma-1) + 2^\alpha((\gamma-1) - 1).$$

Thus

$$M_1^a(T) = M_1^a(T_1) + 2^\alpha \geq (n - \gamma)^\alpha + n - \gamma + 2^\alpha(\gamma - 2) + 2^\alpha.$$

It is easy to check that the bound is satisfied if $\gamma = 1$ and if $\gamma = \frac{n}{2}$. If $\gamma = 1$, we obtain a star and for stars S_n we get $M_1^a(S_n) = (n - 1)^\alpha + n - 1$. If $\gamma = \frac{n}{2}$, then both partite sets of T (which is a bipartite graph) have $\frac{n}{2}$ vertices. Each partite set is a dominating set of T , so there is a dominating set containing the leaf v_1 . Then we can use Case 2 and prove the bound by induction.

Let us show that the bounds are sharp. Let T be a tree containing one vertex w having degree s , where w is adjacent to $n - 2\gamma + 1$ leaves and $\gamma - 1$ vertices of degree 2 such that every vertex of degree 2 is adjacent to a leaf. The vertices of degree at least 2 form a minimum dominating set. The order of T is n and the domination number is γ . We have

$$M_1^a(T) = (n - \gamma)^\alpha + n - \gamma + 2^\alpha(\gamma - 1),$$

therefore the bounds are sharp. □

4. Conclusion

In Theorem 3.1 we showed that if $a > 1$ or $a < 0$, then for a tree T having order n and independence number s , we have

$$M_1^a(T) \geq (n - 1 - (n - s)p)(p + 1)^a + (1 - s + (n - s)p)p^a + (n - s - 1)2^a + 2s - n + 1,$$

where $p = \left\lfloor \frac{n-1}{n-s} \right\rfloor$. Vasilyev, Darda and Stevanović [10] proved that

$$M_1(T) \geq 2(n - 1) + \left\lfloor \frac{n - 1}{s} \right\rfloor (2n - 2 - s) + \left\lfloor \frac{n - 1}{n - s} \right\rfloor (n - 2 + s) - \left\lfloor \frac{n - 1}{s} \right\rfloor^2 s - \left\lfloor \frac{n - 1}{n - s} \right\rfloor^2 (n - s).$$

Note that this result can be presented in a simpler form. For any tree having n vertices and independence number s , we have $\frac{n}{2} \leq s \leq n-1$, therefore $\lfloor \frac{n-1}{s} \rfloor = 1$. For $a = 2$, the zeroth-order general Randić index is the first Zagreb index and from Theorem 3.1 we obtain

$$\begin{aligned} M_1(T) = M_1^2(T) &\geq (n-1 - (n-s)p)(p+1)^2 + (1-s + (n-s)p)p^2 + (n-s-1)2^2 + 2s - n + 1 \\ &= 4(n-1) - 2s + (n+s-2)p - (n-s)p^2 \\ &= 4(n-1) - 2s + \left\lfloor \frac{n-1}{n-s} \right\rfloor (n+s-2) - \left\lfloor \frac{n-1}{n-s} \right\rfloor^2 (n-s). \end{aligned}$$

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