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Extremal First Leap Zagreb Index of k-Generalized Quasi-Trees

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Abstract For a graph G, the first leap Zagreb index is defined as $LM_1(G)=\sum_{v\in V(G)} d_2(v/G)^2$, where $d_2(v/G)$ is the 2-distance degree of a vertex v in G. Let $\mathcal{QT}^{(k)}(n)$ be the set of k-generalized quasi-trees with n vertices. In this paper, we determine the extremal elements from the set $\mathcal{QT}^{(k)}(n)$ with respect to the first leap Zagreb index.

Keywords k-generalized quasi-trees; the first leap Zagreb index; 2-distance degree

MR(2020) Subject Classification 05C30; 05C75; 05C92

1. Introduction

The graph generally means a simple undirected graph G with vertex set $V(G)$ and edge set $E(G)$. We write $|G|$ for the order of G. In this paper, we always consider simple graphs which have no loop or multiple edges. The distance $d(u,v)$ between any two vertices $u,v\in V(G)$, is equal to the length of (number of edges in) a shortest path connecting them. The *eccentricity of* v is defined as $\varepsilon_G(v)=\max\{d(u,v)|u\in V(G)\}$. The diameter of G is $\mathrm{diam}(G)=\max\{\varepsilon_G(v)|v\in V(G)\}$. For a vertex $v\in V(G)$ and a positive integer k, the open k-neighborhood of v in the graph G, denoted by $N_k(v/G)$, is defined as $N_k(v/G)=\{u\in V(G):d(u,v)=k\}$. The k-distance degree of a vertex v in G, denoted by $d_k(v/G)$, is the number of k-neighbors of the vertex v in G, i.e., $d_k(v/G)=|N_k(v/G)|$. For simplicity, write $d_1(v/G)=d(v/G)$ and $N_1(v/G)=N(v/G)$. The degree sequence of G is a sequence of positive integers $\pi=(d_1,d_2,\ldots,d_n)$ if $d_i=d(v_i/G)$ $(i=1,\ldots,n)$ holds, where $V(G)=\{v_1,v_2,\ldots,v_n\}$. The minimum degree in a graph G is denoted by $\delta(G)$.

For a vertex $v\in V(G)$, the graph $G-v$ is a graph obtained from G by removing the vertex v and its incident edges. For any subset $S\subseteq V(G)$, let $G-S$ be the graph obtained from G by removing all the vertices of S and its incident edges. In a graph G, if there exists a vertex $v\in V(G)$ such that $G-v$ is a tree, then such a vertex v is called a quasi vertex and the graph G is called a quasi-tree (or an apex tree). Similarly, a graph G with $|G|=n$ is called a k-generalized

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quasi-tree (or a k-apex tree), if there exists a subset $V_k \subseteq V(G)$ with $|V_k| = k$ such that $G - V_k$ is a tree but for any other subset $V_{k-1} \subseteq V(G)$ with $|V_{k-1}| \leq k-1$, $G - V_{k-1}$ is not a tree. The quasi-tree and the k-generalized quasi-tree were introduced in [1, 2]. In a tree T, deletion of any vertex v with $d(v/T) = 1$ will deduce another tree, which implies that any tree is a quasi-tree. Trees are called trivial quasi-trees and other quasi-trees are called non-trivial quasi-trees. Let $\mathcal{QT}^{(k)}(n)$ be the set of k-generalized quasi-trees with n vertices, where $k \geq 2$. For $k = 1$, we denote by $\mathcal{QT}^{(1)}(n)$ the set of non-trivial quasi-trees of order n. If a, b are two integers with $a \leq b$, we let $[a, b]$ be the set of integers between a and b.

In the interdisciplinary of mathematics, chemistry and physics, molecular invariant could be useful for the study of quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) and for the descriptive presentations of biological and chemical properties, such as boiling and melting points, toxicity, physicochemical and biological properties [3–9]. In 1972, Gutman and Trinajstič [10] introduced the oldest degree based topological index under the name first and second Zagreb index and defined as

$$M_1(G) = \sum_{v \in V(G)} d(v/G)^2,$$

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

In recent years, some novel variants of Zagreb indices have been put forward, such as Zagreb coindices [11–13], reformulated Zagreb indices [14, 15], Zagreb hyperindex [16, 17], multiplicative Zagreb indices [18, 19], multiplicative sum Zagreb index [20, 21], and multiplicative Zagreb coindices [22], etc. In 2017, Naji et al. [23] extended the concept of Zagreb indices to analogous graph invariants based on the second vertex degrees and proposed to name these graph invariants leap Zagreb indices. The first, second and third leap Zagreb index were defined in [23] as follows:

$$LM_1(G) = \sum_{v \in V(G)} d_2(v/G)^2,$$

$$LM_2(G) = \sum_{uv \in E(G)} d_2(u/G)d_2(v/G),$$

$$LM_3(G) = \sum_{v \in V(G)} d(v/G)d_2(v/G).$$

Akhter et al. [24, 25] presented upper and lower bounds on weighted Harary index, Zagreb index, and Randić index of k-generalized quasi-trees. Sharp bounds on first and second multiplicative Zagreb indices for k-generalized quasi-trees has been computed in [26]. Zeroth-order general Randić index of k-generalized quasi-trees has been calculated in [27]. Motivated by these, we describe the upper and the lower bounds for the first leap Zagreb index of k-generalized quasi-trees.

2. The first leap Zagreb index of quasi-trees

In this section, we will give the upper and the lower bounds on the first leap Zagreb index of quasi-trees. Firstly, we calculate the upper and the lower bounds on the first leap Zagreb index of trees. The following two lemmas are useful in the proof of our result.

Lemma 2.1 *$G \in \mathcal{QT}^{(1)}(n)$. $\delta(G) \leq 2$. If $d(v/G) = 1$, then $G - v \in \mathcal{QT}^{(1)}(n-1)$, that is, if $G \in \mathcal{QT}^{(1)}(n)$ and $G - x$ is a tree, then $d(x/G) \geq 2$.*

Proof By way of contradiction, assume that $\delta(G) \geq 3$. Since $G - x$ is a tree, where x is a quasi-vertex of G, $\delta(G - x) = 1$, contradicting $\delta(G) \geq 3$.

Assume that $G - v \notin \mathcal{QT}^{(1)}(n-1)$. Then $G - v$ is a tree. Hence there is no cycle in $G - v$, which implies that G does not contain a cycle. Therefore, G is a tree, a contradiction. This completes the proof of Lemma 2.1. □

Lemma 2.2 *If $G \in \mathcal{QT}^{(k)}(n)$ and $d(v/G) = 1$, then $G - v \in \mathcal{QT}^{(k)}(n-1)$, that is, if $G \in \mathcal{QT}^{(k)}(n)$ and $G - x \in \mathcal{QT}^{(k-1)}(n-1)$, then $d(x/G) \geq 2$.*

Proof We prove the result by induction on k. If $k = 1$, it follows from Lemma 2.1 that the result holds. Assume that the result holds for $k - 1$. We choose a graph $G \in \mathcal{QT}^{(k)}(n)$ and $d(v/G) = 1$. Set $G' = G - v$. By way of contradiction, suppose that $G' \in \mathcal{QT}^{(k-1)}(n-1)$. Hence there is a vertex $x \in V(G)$ with $d(x/G') \geq 2$ such that $G' - x \in \mathcal{QT}^{(k-2)}(n-2)$, that is, $G - x - v \in \mathcal{QT}^{(k-2)}(n-2)$. Set $G'' = G - x$. We claim that $G'' \notin \mathcal{QT}^{(k-1)}(n-1)$. Otherwise, it contradicts the induction hypothesis. If $G'' \in \mathcal{QT}^{(k)}(n-1)$, then $G - x - v \in \mathcal{QT}^{(k-1)}(n-1)$, a contradiction. This completes the proof of Lemma 2.2. □

The next two lemma provide the sharp lower and upper bound on the first leap Zagreb index of trees and characterize the extremal graphs achieving such bound.

Lemma 2.3 *Let T be a tree with $|T| = n$ and $n \geq 4$. Then $LM_1(T) \geq 4n - 12$. Equality holds if and only if T is a path.*

Proof We will prove the theorem by induction on n. If $n = 4$, it is easy to check that $LM_1(T) \geq 4n - 12$. Assume that the result holds for any tree T with $|T| = n - 1$. We will prove the result holds for any tree T with $|T| = n$. For a vertex $v \in V(T)$ with $d(v/T) = 1$, set $T' = T - v$. By the induction hypothesis, we have

$$\begin{aligned} LM_1(T) &\geq LM_1(T') + \sum_{w \in N_2(v/T)} (2d_2(w/T') + 1) + d_2(v/T)^2 \\ &\geq 4(n-1) - 12 + 4 = 4n - 12. \end{aligned}$$

Equality holds if and only if $d_2(v/T) = d_2(w/T') = 1$, that is, T is a path. Hence, Lemma 2.3 is true. □

Lemma 2.4 *Let T be a tree with $|T| = n$. Then $LM_1(T) \leq (n-2)^2(n-1)$ and equality holds if and only if T is a star.*

Proof By way of contradiction, let T be a minimum counter example to Lemma 2.4. Let

$v \in V(T)$ such that $d(v/T) = 1$. Then $LM_1(T - v) \leq (n-3)^2(n-2)$. Set $T' = T - v$.

$$\begin{aligned} LM_1(T) &= LM_1(T') + d_2(v/T)^2 + \sum_{u \in N_2(v/T)} (2d_2(u/T') + 1) \\ &\leq (n-3)^2(n-2) + (n-2)^2 + (n-2)(2(n-3)+1) \\ &= (n-2)^2(n-1), \end{aligned}$$

a contradiction. Hence, Lemma 2.4 is true. □

In the following, we will give the upper and the lower bound of the first leap Zagreb index for quasi-trees.

Theorem 2.5 *Let G be a quasi-tree on n vertices. Then*

$$LM_1(G) \geq \begin{cases} 2, & \text{if } n = 4, \\ 8, & \text{if } n = 5, \\ 12, & \text{if } n = 6, \\ 4n - 10, & \text{if } n \geq 7. \end{cases}$$

Equality holds if and only if $\delta(G) = d(v/G) = 1$ and the degree sequence of G is $(3, \underbrace{2, \ldots, 2}_{n-2}, 1)$.

Proof Assume that $\delta(G) = d(v/G)$ and x is the quasi vertex.

We will prove the theorem by induction on n. If $n \in [4, 6]$, it is easy to check that $LM_1(G) \geq 2$, 8 or 12, respectively. In the following, we may assume that $n \geq 7$ and Theorem 2.5 holds for any graph $G \in \mathcal{QT}^{(1)}(n-1)$. Now we choose $G \in \mathcal{QT}^{(1)}(n)$ such that $LM_1(G)$ is as small as possible. Set $N(v/G) = \{v_1, v_2, \ldots, v_p\}$. Then $p \leq 2$. Let $G' = G - v$.

If G' is not a tree, then $G' \in \mathcal{QT}^{(1)}(n-1)$. By the induction hypothesis, we can get that

$$\begin{aligned} LM_1(G) &\geq LM_1(G') + \sum_{u \in N_2(v/G)} (2d_2(u/G') + 1) + d_2(v/G)^2 \\ &\geq 4(n-1) - 10 + 4 = 4n - 10. \end{aligned}$$

Equality holds if and only if $\delta(G) = d(v/G) = d_2(v/G) = d_2(u/G') = 1$ and the degree sequence of G is $(3, \underbrace{2, \ldots, 2}_{n-2}, 1)$.

If G' is a tree, then $d(v/G) = 2 = \delta(G)$. Suppose that $N(v/G) = \{v_1, v_2\}$. This together with Lemma 2.3, we have

$$\begin{aligned} LM_1(G) &\geq LM_1(G') + \sum_{u \in N_2(v/G)} (2d_2(u/G') + 1) + d_2(v/G')^2 \\ &\geq 4(n-1) - 12 + 5 + 1 \geq 4n - 10. \end{aligned}$$

Equality holds if and only if G' is a path, $d_2(u/G') = 2$ and $d_2(v/G') = 1$. Therefore, the degree sequence of G is $(3, \underbrace{2, \ldots, 2}_{n-2}, 1)$. Hence, Theorem 2.5 is true. □

Lemma 2.6 ([23]) $LM_1(G) \leq M_1(G) + n(n-1)^2 - 4m(n-1)$. *Equalities hold if and only if* *the diameter of G is at most two.*

Lemma 2.7 ([28]) *Let T be a tree on n vertices. Then $M_1(T) \leq n(n-1)$ equality holds if and only if T is a star on n vertices.*

Based on the above two lemmas, we will compute the upper bound of the first leap Zagreb index for quasi-trees.

Lemma 2.8 *Let G be a quasi-tree on n vertices and m edges. Then $M_1(G) + n(n-1)^2 - 4m(n-1) \leq 2(n-3)^2 + (n-3)(n-2)^2$, where $n \geq 4$. Equality holds if and only if the degree sequence of G is $(n-1, 2, 2, \underbrace{1, \ldots, 1}_{n-3})$.*

Proof We will prove the lemma by induction on n. It is easy to check Lemma 2.8 is true if $n = 4$. Suppose that the result holds for any graph $G \in \mathcal{QT}^{(1)}(n-1)$. Now we choose $G \in \mathcal{QT}^{(1)}(n)$. Assume that $\delta(G) = d(v/G)$. By Lemma 2.1, $d(v/G) \leq 2$.

Case 1. $d(v/G) = 1$.

Suppose that $uv \in E(G)$. Then $G' = G - v \in \mathcal{QT}^{(1)}(n-1)$ and $m = m' + 1$, where m' is the number of edges of G'. Hence,

$$
\begin{aligned}
&M_1(G) + n(n-1)^2 - 4m(n-1) \\
&\quad = M_1(G') + 2d(u/G') + 1 + n(n-1)^2 - 4(m'+1)(n-1) + 1 \\
&\quad \leq 2(n-4)^2 + (n-4)(n-3)^2 - (n-1)(n-2)^2 - 4m' - 4(n-1) + 2d(u/G') + 2 + n(n-1)^2 \\
&\quad \leq n^3 - 5n^2 + 4n + 6 = 2(n-3)^2 + (n-3)(n-2)^2.
\end{aligned}
$$

Equality holds if and only if $d(u/G') = n-2$, $m' = n-1$ and the diameter of G is two, that is, the degree sequence of G is $(n-1, 2, 2, \underbrace{1, \ldots, 1}_{n-3})$.

Case 2. $d(v/G) = 2$.

Assume that $vv_1, vv_2 \in E(G)$. Then $m = m' + 2$.

(1) $G' = G - v$ is not a tree. Hence,

$$
\begin{aligned}
&M_1(G) + n(n-1)^2 - 4m(n-1) \\
&\quad = M_1(G') + 2d(v_1/G') + 2d(v_2/G') + 2 + n(n-1)^2 - 4(m'+2)(n-1) + 2^2 \\
&\quad \leq 2(n-4)^2 + (n-4)(n-3)^2 - (n-1)(n-2)^2 + n(n-1)^2 + 2 - 4m' - 8(n-1) + \\
&\qquad 2(d(v_1/G') + d(v_2/G')) + 4.
\end{aligned}
$$

Since $d(v_1/G') + d(v_2/G') \leq m' + 1$, we have

$$M_1(G) + n(n-1)^2 - 4m(n-1) \leq n^3 - 5n^2 + 2n + 14 < n^3 - 5n^2 + 4n + 6.$$

(2) $d(v/G) = 2$ and $T = G - v$ is a tree.

Hence, by Lemma 2.7, we have

$$
\begin{aligned}
&M_1(G) + n(n-1)^2 - 4m(n-1) \\
&\quad = M_1(T) + 2d(v_1/T) + 2d(v_2/T) + 2 + n(n-1)^2 - 4(n-2+2)(n-1) + 2^2
\end{aligned}
$$

$$\begin{aligned}
&\le M_1(T)+2\sum_{i=1}^{2}d(v_i/T)+2+n(n-1)^2-4n(n-1)+2^2\\
&\le (n-1)^2-(n-1)+2(n-1)+2+n(n-1)^2-4n(n-1)+2^2\\
&=2(n-3)^2+(n-3)(n-2)^2.
\end{aligned}$$

Equality holds if and only if $d(v_1/G)+d(v_2/G)=n+1$ and T is a star. This completes the proof of Lemma 2.8. $\square$

Theorem 2.9 *Let G be a quasi-tree. $LM_1(G)\le 2(n-3)^2+(n-3)(n-2)^2$, where $n\ge 4$. Equality holds if and only if the diameter of G is two and the degree sequence G is $(n-1,2,2,\underbrace{1,\ldots,1}_{n-3})$.*

Proof By Lemmas 2.5 and 2.7, Theorem 2.9 is true. Equality holds if and only if the diameter of G is two and the degree sequence of G is $(n-1,2,2,\underbrace{1,\ldots,1}_{n-3})$. $\square$

3. The first leap Zagreb index of k-generalized quasi-trees

In this section, we will compute the upper bounds of the k-generalized quasi-trees for the first leap Zagreb index and the lower bounds of the k-generalized quasi-trees with $k=2$ for the first leap Zagreb index. First, we prove the following lemma, which is useful in the proof of our results.

Lemma 3.1 *Let $G\in\mathcal{QT}^{(2)}(n)$ on n vertices and m edges. Then $M_1(G)+n(n-1)^2-4m(n-1)\le 4(n-3)^2+(n-5)(n-2)^2$. Equality holds if and only if the degree sequence is $(n-1,2,2,2,2,\underbrace{1,\ldots,1}_{n-5})$.*

Proof Since $G\in\mathcal{QT}^{(2)}(n)$, there is a vertex $x_1\in V(G)$ such that $G-x_1\in\mathcal{QT}^{(1)}(n-1)$. Suppose that $G'=G-x_1$ and $N(x_1/G)=\{v_1,\ldots,v_p\}$. Then $m=m'+p$, where m' is the number of edges of G'. Thus, from Lemma 2.8, we have

$$\begin{aligned}
&M_1(G)+n(n-1)^2-4m(n-1)\\
&\quad=M_1(G')+\sum_{i=1}^{p}(2d(v_i/G')+1)+p^2+n(n-1)^2-4(m'+p)(n-1)\\
&\quad\le 2(n-4)^2+(n-4)(n-3)^2-(n-1)(n-2)^2+4m'(n-2)+\\
&\qquad\sum_{i=1}^{p}(2d(v_i/G')+1)+p^2+n(n-1)^2-4(m'+p)(n-1)\\
&\quad\le 2(n-4)^2+(n-4)(n-3)^2-(n-1)(n-2)^2+n(n-1)^2+2^2+\\
&\qquad\sum_{i=1}^{2}(2d(v_i/G')+1)-4m'-8(n-1).
\end{aligned}$$

Since $d(v_1/G') + d(v_2/G') \leq m' + 1$, we have

$$M_1(G) + n(n-1)^2 - 4m(n-1) \leq 4(n-3)^2 + (n-5)(n-2)^2.$$

Equality holds if and only if the degree sequence of G is $(n-1, 2, 2, 2, 2, \underbrace{1, \ldots, 1}_{n-5})$. $\square$

Theorem 3.2 *Let $G \in \mathcal{QT}^{(2)}(n)$. Then $LM_1(G) \leq 4(n-3)^2 + (n-5)(n-2)^2$. Equality holds if and only if the degree sequence of G is $(n-1, 2, 2, 2, 2, \underbrace{1, \ldots, 1}_{n-5})$.*

Proof It follows from Lemmas 2.7 and 3.1 that the result is true and equality holds if and only if the degree sequence of G is $(n-1, 2, 2, 2, 2, \underbrace{1, \ldots, 1}_{n-5})$. $\square$

Theorem 3.3 *Let $G \in \mathcal{QT}^{(k)}(n)$ on n vertices and m edges. Then $M_1(G) + n(n-1)^2 - 4m(n-1) \leq 2k(n-3)^2 + (n-2k-1)(n-2)^2$. Equality holds if and only if the degree sequence of G is $(n-1, \underbrace{2, 2, \ldots, 2}_{2k}, \underbrace{1, \ldots, 1}_{n-2k-1})$.*

Proof We will prove the lemma by induction on k. If $k = 1$, by Lemma 2.8, Theorem 3.3 holds. Suppose that the result holds for any graph $G \in \mathcal{QT}^{(k-1)}(n)$. We choose $G \in \mathcal{QT}^{(k)}(n)$. Assume $x_k \in V(G)$ such that $G' = G - x_k \in \mathcal{QT}^{(k-1)}(n-1)$. Set $N(x_k/G) = \{v_1, \ldots, v_p\}$. Then $p \geq 2$. By the induction hypothesis, we have

$$\begin{aligned}
&M_1(G) + n(n-1)^2 - 4m(n-1) \\
&\leq M_1(G') + \sum_{i=1}^{p}(2d(v_p/G') + 1) + p^2 + n(n-1)^2 - 4(m'+p)(n-1) \\
&\leq 2(k-1)(n-4)^2 + (n-2k)(n-3)^2 - (n-1)(n-2)^2 + 4m'(n-2) + n(n-1)^2 - \\
&\quad 4(m'+p)(n-1) + \sum_{i=1}^{p}(2d(v_i/G') + 1) + p^2 \\
&\leq 2(k-1)(n-4)^2 + (n-2k)(n-3)^2 - (n-1)(n-2)^2 + 4m'(n-2) + n(n-1)^2 - \\
&\quad 4(m'+2)(n-1) + \sum_{i=1}^{2}(2d(v_i/G') + 1) + 2^2.
\end{aligned}$$

Since $d(v_1/G') + d(v_2/G') - 1 \leq m'$, we have

$$M_1(G) + n(n-1)^2 - 4m(n-1) \leq 2k(n-3)^2 + (n-2k-1)(n-2)^2.$$

Equality holds if and only if $p = 2$ and hence the degree sequence of G is $(n-1, \underbrace{2, 2, \ldots, 2}_{2k}, \underbrace{1, \ldots, 1}_{n-2k-1})$. $\square$

Theorem 3.4 *Let $G \in \mathcal{QT}^{(k)}(n)$. Then $LM_1(G) \leq 2k(n-3)^2 + (n-2k-1)(n-2)^2$. Equality holds if and only if the degree sequence is $(n-1, \underbrace{2, \ldots, 2}_{2k}, \underbrace{1, \ldots, 1}_{n-2k-1})$.*

Proof It follows from Lemma 2.8 and Theorem 3.3 that the result holds. Equality holds if and only if the degree sequence is $(n-1,\underbrace{2,\ldots,2}_{2k},\underbrace{1,\ldots,1}_{n-2k-1})$. $\square$

Theorem 3.5 *If $G\in \mathcal{QT}^{(2)}(n)$, then*

$$LM_1(G)\begin{cases} =0, & \text{if } n=3 \text{ or } 4,\\ =2, & \text{if } n=5,\\ =10, & \text{if } n=6,\\ =18, & \text{if } n=7,\\ \geq 4n-6, & \text{if } n\geq 8.\end{cases}$$

Equality holds if and only if $d(v/G)=1$, $q=1$, $d_2(v/G)=1$. And hence the degree sequence of G is $(4,3,3,3,\underbrace{2,2,\ldots,2}_{n-5},1)$.

Proof It is easy to check that the result holds if $n\in[3,8]$. We prove the result by induction on n. Assume that the result holds for any $G\in\mathcal{QT}^{(2)}(n-1)$. We choose $G\in\mathcal{QT}^{(2)}(n)$ such that $LM_1(G)$ is as small as possible. Set $d(v/G)=\delta(G)$ and $G'=G-\{v\}$.

$$\begin{aligned} LM_1(G) &\geq LM_1(G')+\sum_{w\in N_2(v/G)}(2d_2(w/G)+1)+d_2(v/G)^2\\ &\geq 4(n-1)-6+4=4n-6.\end{aligned}$$

Equality holds if and only if $d(v/G)=d_2(v/G)=1$. And hence the degree sequence of G is $(4,3,3,3,\underbrace{2,2,\ldots,2}_{n-5},1)$. $\square$

4. Concluding remarks

We have considered upper/lower bounds for the first leap Zagreb index of k-generalized quasi-trees. The upper bound is determined in terms of number of edges, 2-distance degree and the first Zagreb indices. The lower bound is proved by the inductive method.

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