Zeroth-order general Randić index of $k$-generalized quasi trees

Muhammad Kamran Jamil

Department of Mathematics, Riphah Institute of Computing and Applied Sciences (RICAS),
Riphah International University, 14 Ali Road, Lahore, Pakistan.

Ioan Tomescu

Faculty of Mathematics and Computer Science, University of Bucharest, Romania.

Abstract
For a simple graph $G(V,E)$, the zeroth-order general Randić index is defined as $^{0}R_{\alpha}(G) = \sum_{v \in V(G)} d(v)^{\alpha}$, where $d(v)$ is the degree of the vertex $v$ and $\alpha \neq 0$ is a real number. The $k$-generalized quasi-tree is a connected graph $G$ with a subset $V_{k} \subset V(G)$, where $|V_{k}| = k$ such that $G - V_{k}$ is a tree, but for any subset $V_{k-1} \subset V(G)$ with cardinality $k - 1$, $G - V_{k-1}$ is not a tree. In this paper, we characterize the extremal $k$-generalized quasi trees with the minimum and maximum values of the zeroth-order general Randić index for $\alpha \neq 0$.

Keywords: $k$-generalized quasi tree, zeroth-order general Randić index, extremal graphs.

1. Introduction

Let $G = (V(G), E(G))$ be a simple connected graph, where $V(G)$ and $E(G)$ represent the sets of vertices and edges, respectively. The Randić
index introduced in 1975, is defined as follows:

\[ R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-1/2}, \]

where \( d(v) \) is the degree of the vertex \( v \) in \( G \).

Li et al. proposed the general Randić index by replacing the exponent \(-1/2\) by an arbitrary real number \( \alpha \). This index is defined as

\[ R_\alpha(G) = \sum_{uv \in E(G)} (d(u)d(v))^\alpha. \]

The zeroth-order Randić index, defined by Kier et al. \[8\], is

\[ ^0R_{-1/2}(G) = \sum_{v \in V(G)} d(v)^{-1/2}. \]

The first Zagreb index was introduced by Gutman et al. in 1972 \[5\] and it is defined as

\[ ^0R_2(G) = \sum_{v \in V(G)} d(v)^2. \]

The common generalization of the first Zagreb index and the zeroth-order Randić index was made by Li et al. \[12\]. He proposed the zeroth-order general Randić index \(^0R_\alpha\) by

\[ ^0R_\alpha(G) = \sum_{v \in V(G)} d(v)^\alpha. \]

The above mentioned topological indices have been closely correlated with many physical and chemical properties of the molecules such as boiling point, calculated surface, molecular complexity, heterosystems, chirality, e.g. More information on these indices can be obtained from \[4, 6, 7, 9, 10, 13\].

A graph \( G \) is called a quasi-tree, if there exists a vertex \( z \in V(G) \) such that \( G - z \) is a tree and such a vertex is called a quasi vertex. As deletion of any vertex with degree one will deduce another tree it follows that any tree is a quasi tree. A graph \( G \) is called \( k \)-generalized quasi tree if there exists a subset \( V_k \subset V(G) \) with cardinality \( k \) such that \( G - V_k \) is a tree but for
any subset $V_{k-1} \subset V(G)$ with cardinality $k - 1$, $G - V_{k-1}$ is not a tree. The vertices of $V_k$ are also called quasi vertices (or $k$-quasi vertices). To draw a $k$-generalized quasi tree we need at least $k + 2$ vertices. We call any tree a trivial quasi tree and other quasi trees are called non-trivial quasi trees. We denote the class of $k$-generalized quasi trees of order $n$ by $T_k(n)$.

All graphs considered in this paper are undirected, finite, simple and connected. For terminology and notation not defined here we refer [3]. Let $G$ and $H$ be two vertex disjoint graphs. $G + H$ denotes the join graph of $G$ and $H$ with vertex set $V(G + H) = V(G) \cup V(H)$ and the edge set $E(G + H) = E(G) \cup E(H) \cup \{uv|v \in V(G), v \in V(H)\}$. $S_n$ and $P_n$ represent the star and the path of order $n$, respectively. $S_{p,q}(u,v)$ denotes the bistar of order $p + q$, which is a tree consisting of two adjacent vertices $u$ and $v$, such that $u$ is adjacent to $p - 1$ pendant vertices and $q$ is adjacent to $q - 1$ pendant vertices. If $G$ and $H$ are vertex disjoint graphs and $u, v \in V(H)$, $G \bullet_{u,v} H$ represents the graph having vertex set $V(G) \cup V(H)$ obtained by joining every vertex of $G$ to vertices $u$ and $v$ of $H$.

Akhter et al. [1] found the extremal first and second Zagreb indices of $k$-generalized quasi trees. Qiao [14] determined the extremal $k$-generalized quasi trees, for $k = 1$, with the minimum and maximum values of the zeroth-order general Randić index. In this paper, we characterize the extremal $k$-generalized quasi trees of order $n$ with the maximum and minimum values of the zeroth-order general Randić index for $\alpha \neq 0$. Our results extend the results of Akhter and Qiao.

2. Results and Discussion

In this section, first we will discuss some auxiliary lemmas which will be helpful to prove main results.

Lemma 1. [11] Among all trees with $n$ vertices, the trees with extremal zeroth-order general Randić index are listed in the following table:

Lemma 2. If $u, v \in V(G)$ such that $uv \notin E(G)$, then for $\alpha < 0$

$$^0R_{\alpha}(G + uv) < ^0R_{\alpha}(G),$$

and for $\alpha > 0$

$$^0R_{\alpha}(G + uv) > ^0R_{\alpha}(G).$$
| minimum          | 0 < \(\alpha\) < 1 | \(\alpha\) < 0 or \(\alpha\) > 1 |
|------------------|---------------------|----------------------------------|
| trees with \([3, 2^{n-4}, 1^4]\) | trees with \([3^2, 2^{n-6}, 1^4]\) | the path \(P_n\) |
| second minimum   | the double star \(S_{n-2,2}\) | the star \(S_n\) |
| third minimum    | the double star \(S_{n-3,3}\) | the path \(P_n\) |
| maximum          | the double star \(S_{n-2,2}\) | trees with \([3, 2^{n-4}, 1^4]\) |
| second maximum   | trees with \([3^2, 2^{n-6}, 1^4]\) | trees with \([3^2, 2^{n-6}, 1^4]\) |
| third maximum    | the double star \(S_{n-3,3}\) | trees with \([3^2, 2^{n-6}, 1^4]\) |

**Lemma 3.** Let \(G \in T_k(n)\). If \(^0R_\alpha(G)\) is minimum (maximum) and \(z\) is a quasi vertex of \(G\), then \(d(z) = n - 1\) for \(\alpha < 0\) (\(\alpha > 0\), respectively).

**Proof.** Let \(G \in T_k(n)\), \(^0R_\alpha(G)\) be minimum (maximum) and \(z\) be a quasi vertex of \(G\). Suppose on contrary \(d(z) < n - 1\), then there is a vertex \(x \in V(G)\) such that \(xz \notin E(G)\). Now \(G + xz\) is also in \(T_k(n)\) and \(^0R_\alpha(G + xz) < ^0R_\alpha(G)\) for \(\alpha < 0\) \((^0R_\alpha(G + xz) > ^0R_\alpha(G)\) for \(\alpha > 0\)), a contradiction, hence \(d(z) = n - 1\).

**Lemma 4.** Let \(f(x) = x^\alpha - (x + 1)^\alpha\), where \(x > 0\). \(f(x)\) is strictly increasing for \(0 < \alpha < 1\) and strictly decreasing for \(\alpha < 0\) or \(\alpha > 1\).

**Lemma 5.** Let \(G\) be a graph, and \(u, v\) and \(w\) be three vertices of \(G\) such that \(uw \notin E(G)\), \(vw \in E(G)\) and \(d(u) \geq d(v)\). Let \(G' = G + uw - vw\). If \(\alpha < 0\) or \(\alpha > 1\) then \(^0R_\alpha(G') > ^0R_\alpha(G)\) and if \(0 < \alpha < 1\) then \(^0R_\alpha(G') < ^0R_\alpha(G)\).

**Proof.** Let \(d(u) = x\) and \(d(v) = y\). We obtain \(^0R_\alpha(G') - ^0R_\alpha(G) = (x + 1)^\alpha + (y - 1)^\alpha - x^\alpha - y^\alpha = f(y - 1) - f(x)\), where \(f(x) = x^\alpha - (x + 1)^\alpha\). \(f(x)\) is a strictly decreasing function for \(x > 0\) and \(\alpha < 0\) or \(\alpha > 1\). Since \(y - 1 < x\) it follows that \(^0R_\alpha(G') > ^0R_\alpha(G)\). If \(0 < \alpha < 1\) the proof is similar.

**Lemma 6.** Let \(G \in T_k(n)\). If \(^0R_\alpha(G)\) is maximum (minimum) then there exists a spanning subgraph \(H\) of \(G\) such that \(^0R_\alpha(G) \leq ^0R_\alpha(H)\) \(^0R_\alpha(G) \geq ^0R_\alpha(H)\) and for any quasi vertex \(z\) of \(G\) we have \(d_G(z) \geq d_H(z) = 2\) and \(z\) is adjacent in \(H\) to other two vertices which are not quasi vertices for \(\alpha < 0\) (\(\alpha > 0\), respectively).

**Proof.** By definition of a \(k\)-generalized quasi tree, there exists a subset \(X \subset V(G)\) of cardinality \(k\) such that \(G - X\) is a tree and for any \(Y \subset V(G)\) and \(|Y| < k\), \(G - Y\) is not a tree. It follows that \(d(z) \geq 2\) for any vertex \(z \in X\).
If $m$ denotes the number of edges of $G$, then $m \geq 2k + n - k - 1 = n + k - 1$ and equality holds if and only if $d(z) = 2$ for any vertex $z \in X$ and no two vertices in $X$ are adjacent. By Lemma 2 by deleting some edges it follows the existence of the graph $H$, which is not necessarily in $T_k(n)$.

**Lemma 7.** Let $n, x_i (1 \leq i \leq n), p, m \geq 1$ be integers, $\alpha$ be any real number such that $\alpha \notin \{0, 1\}$ and $x_1 + x_2 + \cdots + x_n = p$.

a) The function $f(x_1, x_2, \ldots, x_n; p) = \sum_{i=1}^{n} x_i^\alpha$ is minimum for $\alpha < 0$ or $\alpha > 1$ (maximum for $0 < \alpha < 1$, respectively) if and only if $x_1, x_2, \ldots, x_n$ are almost equal, or $|x_i - x_j| \leq 1$ for every $i, j = 1, 2, \ldots, n$.

b) If $x_1 \geq x_2 \geq m$, the maximum of the function $f(x_1, \ldots, x_n)$ is reached for $\alpha < 0$ or $\alpha > 1$ (minimum for $0 < \alpha < 1$, respectively) only for $x_1 = p - m - n + 2, x_2 = m, x_3 = x_4 = \ldots = x_n = 1$. The second maximum (the second minimum, respectively) is attained only for $x_1 = p - m - n + 1, x_2 = m + 1, x_3 = x_4 = \ldots = x_n = 1$.

**Proof.** We shall consider only the case $\alpha < 0$ or $\alpha > 1$, the proof in the other case being similar.

a) The function $f(x) = x^\alpha - (1 + x)^\alpha$ is a strictly decreasing function for $x > 0$ and $\alpha > 1$ or $\alpha < 0$. If $x \geq y + 2 > 0$ we deduce $x - 1 > y$, which implies $f(x - 1) < f(y)$, or $x^\alpha + y^\alpha > (x - 1)^\alpha + (y + 1)^\alpha$. It follows that $f(x_1, x_2, \ldots, x_n; p) = \sum_{i=1}^{n} x_i^\alpha$ is minimum if and only if $x_1, x_2, \ldots, x_n$ are almost equal.

b) If $x \geq y \geq 2$ then $x > y - 1$, which implies $f(y - 1) > f(x)$, or $(x + 1)^\alpha + (y - 1)^\alpha > x^\alpha + y^\alpha$.

3. Case $\alpha < 0$

**Theorem 8.** Let $G \in T_k(n)$, where $k \geq 1$ and $n \geq 3$. For $\alpha < 0$ we have

$$0^\alpha R_\alpha(G) \geq k(n - 1)^\alpha + 2(k + 1)^\alpha + (n - k - 2)(k + 2)^\alpha$$

and equality holds if and only if $G = K_k + P_{n-k}$.

**Proof.** Suppose that $G \in T_k(n)$ has minimum $0^\alpha R_\alpha(G)$. Let $V_k \subset V(G)$ be the set of $k$-quasi vertices. As $0^\alpha R_\alpha(G + uv) < 0^\alpha R_\alpha(G)$ for any $uv \notin E(G)$, this implies that $V_k$ forms a complete graph in $G$. Then by Lemma 3 we have
\[ G = K_k + T_{n-k}, \text{ where } T_{n-k} \text{ is a tree of order } n - k. \] We can write:

\[
\begin{align*}
0^R_\alpha(G) &= 0^R_\alpha(K_k + T_{n-k}) \\
&= \sum_{v \in V(K_k)} (d(v) + n - k)^\alpha + \sum_{v \in V(T_{n-k})} (d(v) + k)^\alpha \\
&= k(n - 1)^\alpha + \sum_{v \in V(T_{n-k})} (d(v) + k)^\alpha.
\end{align*}
\]

We get

\[
\sum_{v \in V(T_{n-k})} (d(v) + k) = 2(n - k - 1) + k(n - k).
\]

By Lemma 7, \[ \sum_{v \in V(T_{n-k})} (d(v) + k)^\alpha \] is minimum if and only if the degrees of \( T_{n-k} \) are almost equal. Since every tree has at least two vertices of degree one, it follows that the minimum of this sum is reached if and only if \( T_{n-k} \) has two vertices of degree one and \( n - k - 2 \) vertices of degree 2, or \( T_{n-k} = P_{n-k} \).

Finally,

\[
0^R_\alpha(G) \geq k(n - 1)^\alpha + 2(k + 1)^\alpha + (n - k - 2)(k + 2)^\alpha.
\]

Equality holds if and only if \( G = K_k + P_{n-k} \).

**Theorem 9.** Let \( G \in T_k(n) \), where \( n \geq 3 \) and \( k \geq 1 \). If \( \alpha < 0 \) we have:

a) If \( k = 1 \) then

\[
0^R_\alpha(G) \leq (n - 1)^\alpha + 2^{\alpha+1} + n - 3
\]

and equality holds if and only if \( G = K_1 \bullet_{u,v} S_{n-1} \), where \( u \) is the center of \( S_{n-1} \) and \( v \) is a pendant vertex of \( S_{n-1} \).

b) If \( n \geq 4 \) and \( k \geq 2 \) then

\[
0^R_\alpha(G) \leq (n - 2)^\alpha + k2^\alpha + (k + 2)^\alpha + n - k - 2
\]

and equality holds if and only if \( G = \overline{K_k} \bullet_{u,v} S_{n-k-2,2}(u,v) \), where \( u \) and \( v \) are vertices of degree \( n - k - 2 \) and 2 of \( S_{n-k-2,2}(u,v) \), respectively.

**Proof.** Suppose that \( G \in T_k(n) \) has maximum \( 0^R_\alpha(G) \). Let \( V_k \subset V(G) \) be the set of \( k \)-quasi vertices. The graph \( G - V_k \) is a tree of order \( n - k \), denoted by \( T_{n-k} \). As \( 0^R_\alpha(G - uv) \geq 0^R_\alpha(G) \) for any \( uv \in E(G) \), and by Lemmas 5 and 6 we deduce the existence of a graph \( F \) with \( V(F) = V(G) \), \( 0^R_\alpha(G) \leq 0^R_\alpha(F) \) and such that in \( F \) we have: \( V_k \) forms an empty graph,
i.e., it induces $\overline{K}_k$, every quasi vertex of $G$ has degree 2 and quasi vertices have common neighbors $y_1, y_2 \in V(G)$, where $y_1$ is a vertex of maximum degree in $T_{n-k}$ and $y_2$ is a vertex of maximum degree in $T_{n-k} - y_1$. We can represent the graph $F$ as $F = \overline{K}_k \cdot y_1, y_2 T_{n-k}$. We deduce:

$$0^R \alpha(G) = 0^R \alpha(\overline{K}_k \cdot y_1, y_2 T_{n-k}) = \sum_{v \in V(\overline{K}_k \cdot y_1, y_2 T_{n-k})} d(v)^\alpha$$

$$= \sum_{v \in V(\overline{K}_k)} d(v)^\alpha + \sum_{v \in V(T_{n-k}) \setminus y_1, y_2} d(v)^\alpha + (d(y_1) + k)^\alpha + (d(y_2) + k)^\alpha.$$  

We have

$$\sum_{v \in V(T_{n-k}) \setminus y_1, y_2} d(v) + d(y_1) + k + d(y_2) + k = 2n - 2.$$

By Lemma[7] the sum

$$\sum_{v \in V(T_{n-k}) \setminus y_1, y_2} d(v)^\alpha + (d(y_1) + k)^\alpha + (d(y_2) + k)^\alpha \quad (1)$$

is maximum only if $T_{n-k} = S_{n-k}$ and $y_1$ and $y_2$ are the center and a pendant vertex of $S_{n-k}$, respectively. For $k = 1$ this graph is a $k$-generalized quasi-tree, but for $k \geq 2$ this property is no longer valid. We must consider the second maximum of (1). This time $F \in T_k(n), G = F$ and $T_{n-k} = S_{n-k-2}(u, v), y_1 = u$ and $y_2 = v$. The conclusion follows.

4. Case $\alpha \geq 1$

**Theorem 10.** Let $G \in T_k(n), k \geq 1$ and $n \geq 3$, then for $\alpha = 1$

$$2(n + k - 1) \leq 0^R \alpha(G) \leq 2n(k + 1) - k(k + 3) - 2.$$

Left equality holds if and only if $G$ consists of $\overline{K}_k$, a tree $T_{n-k}$ of order $n-k$, every vertex of $\overline{K}_k$ being adjacent to two arbitrary vertices of $T_{n-k}$ such that the resulting graph belongs to $T_k(n)$ and the right equality holds if and only if $G = K_k + T_{n-k}$.

**Proof.** For $\alpha = 1$ we have $0^R \alpha(G) = \sum_{v \in V(G)} d(v) = 2|E(G)| \geq 2(n+k-1)$ and equality holds if and only if the degree of every quasi vertex is two. Hence, the left hand inequality.

Similarly, $|E(G)|$ is maximum only if $G = K_k + T_{n-k}$ and the right hand inequality follows.
Theorem 11. Let $G \in T_k(n)$ and $k \geq 1$, $n \geq 3$, $\alpha > 1$ then

$$(n - 2k + 2)2^\alpha + (2k - 2)3^\alpha \leq 0^\alpha R_\alpha(G) \leq (k + 1)(n - 1)^\alpha + (n - k - 1)(k + 1)^\alpha.$$ 

The upper bound is an equality if and only if $G = K_k + S_{n-k}$.

PROOF. Suppose that $G \in T_k(n)$ has maximum $0^\alpha R_\alpha(G)$. Let $V_k \subset V(G)$ be the set of $k$-quasi vertices. As $0^\alpha R_\alpha(G + uv) > 0^\alpha R_\alpha(G)$ for any $uv \notin E(G)$, this implies that $V_k$ induces a complete subgraph in $G$. Then by Lemma 3 we have $G = K_k + T_{n-k}$, where $T_{n-k}$ is a tree of order $n - k$. It follows that:

$$0^\alpha R_\alpha(G) = 0^\alpha R_\alpha(K_k + T_{n-k})$$

$$= \sum_{v \in V(K_k)} (d(v) + n - k)^\alpha + \sum_{v \in V(T_{n-k})} (d(v) + k)^\alpha$$

$$= k(n - 1)^\alpha + \sum_{v \in V(T_{n-k})} (d(v) + k)^\alpha$$

$$\leq (k + 1)(n - 1)^\alpha + (n - k - 1)(k + 1)^\alpha.$$ 

By Lemma 7 the upper bound is an equality if and only if $T_{n-k} = S_{n-k}$, i.e., $G = K_k + S_{n-k}$.

Suppose now that $0^\alpha R_\alpha(G)$ is minimum. By Lemma 6 there exists a spanning subgraph $H$ of $G$ such that $0^\alpha R_\alpha(G) \geq 0^\alpha R_\alpha(H)$ and every quasi vertex $z$ has $d_H(z) = 2$, being adjacent in $H$ to two vertices which are not quasi vertices, which implies that $\sum_{v \in V(G)} d_H(v) = 2(n + k - 1)$. By Lemma 7 $0^\alpha R_\alpha(H)$ is minimum if the degrees of $H$ are almost equal. We deduce that in this case the degrees of $H$ are equal to 2 or to 3. By denoting $n_i$ the number of vertices having degree $i$ we can write $2n_2 + 3(n - n_2) = 2n + 2k - 2$, which implies $n_2 = n - 2k + 2$ and $n_3 = n - n_2 = 2k - 2$ and yields the lower bound. Consequently, the minimum of $0^\alpha R_\alpha(G)$ is reached if and only if there exist $n - 2k + 2$ vertices (including quasi vertices) of degree 2 and $2k - 2$ vertices of degree 3 (in this case $H = G$). Such a graph is illustrated in Fig. 1. Note that for $k = 1$ we have $n_2 = n$ and $n_3 = 0$, hence $G = C_n$, the cycle with $n$ vertices.

5. Case $0 < \alpha < 1$

By similar methods as in preceding sections we can deduce the extremal values of $0^\alpha R_\alpha(G)$ for $0 < \alpha < 1$ as follows:
Figure 1: k-generalized quasi tree with almost equal vertices degree.

Theorem 12. Let $G \in T_k(n)$, $k \geq 1$ and $n \geq 3$. If $0 < \alpha < 1$ then

$$0^R\alpha(G) \leq k(n-1)^\alpha + 2(k+1)^\alpha + (n-k-2)(k+2)^\alpha.$$

Equality holds if and only if $G = K_k + P_{n-k}$.

Theorem 13. Let $G \in T_k(n)$, where $n \geq 3$ and $k \geq 1$. If $0 < \alpha < 1$ we have:

a) If $k = 1$ then

$$0^R\alpha(G) \geq (n-1)^\alpha + 2^{\alpha+1} + n - 3$$

and equality holds if and only if $G = \overline{K_1} \bullet_{u,v} S_{n-1}$, where $u$ is the center of $S_{n-1}$ and $v$ is a pendant vertex of $S_{n-1}$.

b) If $n \geq 4$ and $k \geq 2$ then

$$0^R\alpha(G) \geq (n-2)^\alpha + k2^\alpha + (k+2)^\alpha + n - k - 2$$

and equality holds if and only if $G = \overline{K_k} \bullet_{u,v} S_{n-k-2}(u,v)$, where $u$ and $v$ are vertices of degree $n-k-2$ and 2 of $S_{n-k-2}(u,v)$, respectively.

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