U.P.B. Sci. Bull., Series A, Vol. 82, Iss. 2, 2020 ISSN 1223-7027

EXTREMAL k-GENERALIZED QUASI TREES FOR GENERAL SUM-CONNECTIVITY INDEX

Muhammad Kamran Jamil[1], Ioan Tomescu[2], Muhammad Imran[3]

For a simple graph G, the general sum-connectivity index is defined as $\chi_\alpha(G) = \sum_{uv\in E(G)}(d(u) + d(v))^\alpha$, where $d(u)$ is the degree of the vertex u 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 have determined sharp upper and lower bounds of the general sum-connectivity index for $\alpha \geq 1$. The corresponding extremal k-generalized quasi trees are also characterized in each case.

Keywords: Extremal graphs, general sum-connectivity index, k-quasi trees
MSC2010: 05C35.

1. Introduction

All graphs considered in this paper are undirected, finite, simple and connected. Let $G = (V(G), E(G))$ be such a graph, where $V(G)$ is the set of vertices and $E(G)$ the set of edges. The number of vertices adjacent to a vertex v in graph G is known as the degree of v, denoted by $d_G(v)$. The set of vertices adjacent with v is denoted by $N(v)$. The distance, denoted by $d(u, v)$, between two vertices $u, v \in V(G)$ is the length of a shortest path between them and the eccentricity of a vertex u, denoted by $ecc(u)$, is the maximum distance $\max\limits_{v\in V(G)} d(u, v)$ from u to any other vertex. The diameter of G, denoted by $diam(G)$, is $\max\limits_{u\in V(G)} ecc(u) = \max\limits_{u,v\in V(G)} d(u, v)$.
S_n represents the star of order n also denoted by $K_{1,n-1}$ and P_n the path with n vertices. $S_{a,b}$ denotes the bistar of order $a + b$, which is a tree consisting of two adjacent vertices u and v, such that u is adjacent to $a - 1$ pendant vertices and b is adjacent to $b - 1$ pendant vertices. Let T be a tree. If $diam(T) = 2$ then T is a star; if $diam(T) = 3$ then T is a double star. 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 $E(G + H) = E(G) \cup E(H) \cup \{uv|v \in V(G), v \in V(H)\}$.

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 yield 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

[1]Department of Mathematics, Riphah Institute of Computing and Applied Sciences, Riphah International University, Lahore, Pakistan., e-mail: m.kamran.sms@gmail.com
[2]Faculty of Mathematics and Computer Science, University of Bucharest, Bucharest, Romania.
[1,3]Department of Mathematical Sciences, United Arab Emirates University, Al Ain, United Arab Emirates.

n by $T_k(n)$.
For terminology and notation not defined here we refer [2].

The first Zagreb index was introduced by Gutman et al. in 1972 [4] and it is defined as

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

A variant of Randić index is known as general sum-connectivity index and was defined [11] as

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d(u) + d(v))^\alpha.$$

Note that $M_1(G) = \chi_1(G)$.

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 [3, 7, 8, 9].
Jamil et al. [6] investigated the extremal k-generalized graphs for zeroth order general Randić index. Akhter et al. [1] found the extremal first and second Zagreb indices of k-generalized quasi trees. Qiao [10] 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 have determined sharp upper and lower bounds of the general sum-connectivity index for $\alpha > 1$ and have characterized the corresponding extremal k-generalized quasi trees in each case, thus extending some results from [1] which hold for $\alpha = 1$.

2. **Main Results**

We start this section by some lemmas that will help to prove the main results.

Lemma 2.1. *Let $u, v \in V(G)$ such that $uv \notin E(G)$, then*

$$\chi_\alpha(G) < \chi_\alpha(G + uv).$$

Lemma 2.2. *Let $G \in T_k(n)$. If $\chi_\alpha(G)$ is maximum and v is a quasi vertex of G then $d(v) = n - 1$.*

Proof. Let $G \in T_k(n)$, $\chi_\alpha(G)$ be maximum and v be a quasi vertex of G. Suppose on contrary $d(v) < n-1$, then there is a vertex $u \in V(G)$ such that $uv \notin E(G)$. Now $G+uv$ is also in $T_k(n)$ and $\chi_\alpha(G + uv) > \chi_\alpha(G)$, a contradiction, hence $d(v) = n - 1$.

For $\alpha > 1$ consider the function $S(x_1, \ldots, x_m) = \sum_{i=1}^m x_i^\alpha$ defined for $(x_1, \ldots, x_m) \in D_{m,p}$, where $D_{m,p}$ is the set of all vectors $(x_1, \ldots, x_m)$ with positive integers coordinates such that $x_1 \geq x_2 \geq \ldots x_m \geq 1$ and $\sum_{i=1}^m x_i = p$. If $1 \leq i < j \leq m$ and $x_j \geq 2$ we replace $(x_1, \ldots, x_m)$ by $(x_1, \ldots, x_i + 1, \ldots, x_j - 1, \ldots, x_m)$. By reordering in decreasing order the components of this vector we get the vector $(x_1^*, \ldots, x_m^*) \in D_{m,p}$, which will be denoted by $\mathbf{z}$. This transformation of $(x_1, \ldots, x_m)$ to $\mathbf{z}$ will be denoted by M_1.
We have $S(\mathbf{z}) - S(x_1, \ldots, x_m) = (x_i + 1)^\alpha + (x_j - 1)^\alpha - x_i^\alpha - x_j^\alpha$.
The function $\phi(x) = x^\alpha - (1 + x)^\alpha$ is a strictly decreasing function for $x > 0$ and $\alpha > 1$. Since $i < j$ implies $x_i \geq x_j$, it follows that $x_j - 1 < x_i$, which implies $\phi(x_j - 1) > \phi(x_i)$, or $(x_i + 1)^\alpha + (x_j - 1)^\alpha > x_i^\alpha + x_j^\alpha$. We get $S(\mathbf{z}) - S(x_1, \ldots, x_m) > 0$. This leads to the following property:

Lemma 2.3. *If there exist $2 \leq j \leq m$ with $x_j \geq 2$ then $S(x_1, \ldots, x_m)$ can be strictly increased on $D_{m,p}$ for $\alpha > 1$.*

Roughly speaking, function S can be strictly increased if we can push one unity to the left in the degree sequence ordered in decreasing order using M_1 transform.

Lemma 2.4. *Let $k \geq 1$, $G \in T_k(n)$. If $\chi_\alpha(G)$ is minimum and v is a quasi vertex, $v \in V_k$, then $d(v) = 2$.*

Proof. Let $G \in T_k(n)$ and $\chi_\alpha(G)$ be as small as possible. If $d(v)$=1 then v cannot be a quasi vertex. Suppose that $d(v) > 2$. Then there exist more than two vertices in G which are adjacent with v. Therefore, for any edge $uv \in E(G)$, $\chi_\alpha(G) > \chi_\alpha(G - uv)$ and $G - uv \in T_k(n)$, which is a contradiction. It follows that $d(v) = 2$. Note that in this case v is adjacent to two vertices belonging to $V - V_k$ since otherwise, by denoting $V_{k-1} = V_k - \{v\}$ we would have that $G - V_{k-1}$ is a tree.

Let G be a graph such that every vertex of G has a fixed weight $w \geq 1$, then we define

$$\chi_{\alpha,w}(G) = \sum_{uv \in E(G)} (d(u) + d(v) + 2w)^\alpha.$$

Lemma 2.5. *For $\alpha > 1$ and $w \geq 1$, the unique tree of order n with the maximum value of $\chi_{\alpha,w}(G)$ is the star S_n.*

Proof. Let T be a tree but not a star or a double star and having maximum $\chi_{\alpha,w}(G)$. It follows that T has diameter $diam(T) \geq 4$. Consequently, there exist vertices u, t and v such that $ut, tv \in E(T)$ with $d_T(u) = a$, $d_T(t) = c$ and $d_T(v) = b$ such that $a, b \geq 2$. Without loss of generality we can suppose that $a \geq b$. Let $N(u) - t = \{u_1, u_2, \cdots, u_{a-1}\}$ and $N(v) - t = \{v_1, v_2, \cdots, v_{b-1}\}$. As in [5] we construct a new graph T' by deleting the edges $vv_1, vv_2, \cdots, vv_{b-1}$ and inserting the new edges $uv_1, uv_2, \cdots, uv_{b-1}$. Considering the values of $\chi_{\alpha,w}$ for T and T', we have

$$\chi_{\alpha,w}(T') - \chi_{\alpha,w}(T) = \sum_{i=1}^{a-1}(a + b + d(u_k) + 2w - 1)^\alpha$$

$$+ \sum_{i=1}^{b-1}(a + b + d(v_k) + 2w - 1)^\alpha + (a + b + c + 2w - 1)^\alpha$$

$$+(c + 2w + 1)^\alpha - \sum_{i=1}^{a-1}(a + d(u_k) + 2w)^\alpha - \sum_{i=1}^{b-1}(b + d(v_k) + 2w)^\alpha$$

$$-(a + c + 2w)^\alpha - (b + c + 2w)^\alpha > (a + b + c + 2w - 1)^\alpha + (c + 2w + 1)^\alpha$$

$$-(a + c + 2w)^\alpha - (b + c + 2w)^\alpha > 0.$$

The last inequality follows from Lemma 2.3 for $m = 2$, $x_1 = a + c + 2w, x_2 = b + c + 2w$, $p = a + b + 2c + 4w$, applying several times transformation M_1. This contradicts the maximality of $\chi_{\alpha,w}(G)$. It remains to show that for any $a, b \geq 2$ and $a + b = n$ we have $\chi_{\alpha,w}(S_n) > \chi_{\alpha,w}(S_{a,b})$. We get

$$\chi_{\alpha,w}(S_n) = (n - 1)(n + 2w)^\alpha$$

$$\chi_{\alpha,w}(S_{a,b}) = (a - 1)(a + 1 + 2w)^\alpha + (b - 1)(b + 1 + 2w)^\alpha + (n + 2w)^\alpha.$$

Their difference is equal to:

$$\chi_{\alpha,w}(S_n) - \chi_{\alpha,w}(S_{a,b}) = (n - 2)(n + 2w)^\alpha - (a - 1)(a + 1 + 2w)^\alpha - (b - 1)(b + 1 + 2w)^\alpha > 0$$

since $a < n - 1, b < n - 1$ imply $a + 1 + 2w < n + 2w$ and $b + 1 + 2w < n + 2w$ and $\alpha > 1$.

Theorem 2.1. *Let $G \in T_k(n)$, where $k \geq 1$ and $n \geq 5$. For $\alpha \geq 1$ we have*

$$\chi_\alpha(G) \leq 2^{\alpha-1}k(k+1)(n-1)^\alpha + (k+1)(n-k-1)(n+k)^\alpha$$

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

Proof. The case $\alpha = 1$ was settled in [1], so we will consider $\alpha > 1$ in what follows. Suppose that $G \in T_k(n)$ has maximum $\chi_\alpha(G)$. Let $V_k \subset V(G)$ be the set of quasi vertices. Then by Lemmas 2.1 and 2.2 we have $G = K_k + T_{n-k}$, where T_{n-k} is a tree with $n-k$ vertices. We shall prove that $T_{n-k} = S_{n-k}$.
It follows that

$$\begin{aligned}
\chi_\alpha(G) &= \chi_\alpha(K_k + T_{n-k}) \\
&= \sum_{uv \in E(K_k)} (d_G(u) + d_G(v))^\alpha + \sum_{u \in V(K_k), v \in V(T_{n-k})} (d_G(u) + d_G(v))^\alpha \\
&+ \sum_{uv \in E(T_{n-k})} (d_G(u) + d_G(v))^\alpha \\
&= k(k-1)2^{\alpha-1}(n-1)^\alpha + k \sum_{v \in V(T_{n-k})} (d_{T_{n-k}}(v) + n + k - 1)^\alpha \\
&+ \sum_{uv \in E(T_{n-k})} ((d_{T_{n-k}}(u) + d_{T_{n-k}}(v) + 2k)^\alpha.
\end{aligned}$$

By Lemma 2.3 the maximum of the sum $\sum_{v \in V(T_{n-k})}(d_{T_{n-k}}(v) + n - 1)^\alpha$ is achieved if and only if the degree sequence of the tree T_{n-k} is $(n-k-1, 1, \ldots, 1)$, i.e., $T_{n-k} = S_{n-k}$. Similarly, by Lemma 2.5 the sum $\sum_{uv \in E(T_{n-k})}((d_{T_{n-k}}(u) + d_{T_{n-k}}(v) + 2k)^\alpha = \chi_{\alpha,k}(T_{n-k})$ is maximized only for $T_{n-k} = S_{n-k}$. Consequently, $G = K_k + S_{n-k}$ and $\chi_\alpha(K_k + S_{n-k}) = 2^{\alpha-1}k(k+1)(n-1)^\alpha + (k+1)(n-k-1)(n+k)^\alpha$.

Theorem 2.2. *Let $\alpha > 1$ and $G \in T_k(n)$.*
(i) If $k = 1$ and $n \geq 3$ then $\chi_\alpha(G) \geq n4^\alpha$ and the equality holds if and only if G is a cycle with n vertices, i.e., $G = C_n$.
(ii) If $k = 2$ and $n \geq 4$ then: $\chi_\alpha(G) \geq 4 \cdot 5^\alpha + 6^\alpha$ for $n = 4$ and $\chi_\alpha(G) \geq (n-5)4^\alpha + 6 \cdot 5^\alpha$ for $n \geq 5$. Equality holds if and only if G consists of two cycles of length three having a common edge for $n = 4$ or two cycles having a common path of length at least two for $n \geq 5$ or two cycles joined by a path of length at least two for $n \geq 7$.

Proof. Let $G \in T_k(n)$ such that $\chi_\alpha(G)$ is as small as possible. If V_k is a set of quasi vertices of G, $G - V_k$ will be a tree of order $n-k$ and by Lemma 2.4, we deduce that $d(x) = 2$ for all $x \in V_k$. Moreover, for every vertex $x \in V_k$, x is adjacent to two vertices from $V - V_k$. This implies that G is connected and has $n+k-1$ edges. It follows that G has k cycles. We shall prove first that G cannot contain pendant vertices. Suppose that G would contain a vertex z such that $d(z) = 1$. In this case there exists a path $z, y, \ldots, w$ joining z to a vertex w which belongs to a cycle, denoted by C of G. Suppose that the vertices, different from z, which are adjacent to y are $z_1, z_2, \ldots, z_t$ and their degrees are $d(z_i) = w_i$ for $1 \leq i \leq t$. We have $d_G(y) = t + 1$. It follows that $t \geq 1$ and at least one degree w_i is greater than or equal to two. We shall define a new k-cyclic graph of order n, denoted by G_1, which is obtained by deleting the edge zy and inserting z between two consecutive vertices, u and v of C. Denote $d_G(u) = a$ and $d_G(v) = b$, where $a, b \geq 2$. We get $d_{G_1}(y) = t$, $d_{G_1}(u) = a$, $d_{G_1}(v) = b$, $d_{G_1}(z) = 2$ and $d_{G_1}(z_i) = w_i$ for each $1 \leq i \leq t$. We deduce that the difference,

$\chi_\alpha(G) - \chi_\alpha(G_1)$, which will be denoted by Δ, is equal to:

$$\Delta = \sum_{i=1}^{t}(t+1+w_i)^\alpha + (t+2)^\alpha + (a+b)^\alpha$$
$$- \sum_{i=1}^{t}(t+w_i)^\alpha - (a+2)^\alpha - (b+2)^\alpha$$
$$= \sum_{i=1}^{t}((t+1+w_i)^\alpha - (t+w_i)^\alpha) + (t+2)^\alpha$$
$$+ (a+b)^\alpha - (a+2)^\alpha - (b+2)^\alpha.$$

If $t \geq 2$ then $\sum_{i=1}^{t}((t+1+w_i)^\alpha - (t+w_i)^\alpha) > 0$ and $(t+2)^\alpha \geq 4^\alpha$. Using Lemma 2.3 we deduce that $(a+b)^\alpha + 4^\alpha - (a+2)^\alpha - (b+2)^\alpha \geq 0$ with equality only for $a = 2$ or $b = 2$. Consequently, $\Delta > 0$, a contradiction.

It follows that $t = 1$. In this case the vertex y is a pendant vertex of G_1. By repeating this procedure with y instead of z and so on we shall find a k-cyclic graph of order n having a pendant vertex adjacent to a vertex w on C. In this case $d(w) \geq 3$, thus implying that corresponding $t \geq 2$ and $\Delta \geq 1$, a contradiction. Suppose now that all vertices of G have their degrees greater than or equal to two.

(i) If $k = 1$, then G has n edges this implies that G is a connected unicyclic graph without pendant vertices. Since $\chi_\alpha(G)$ is minimal and G cannot have pendant vertices we get $G = C_n$.

(ii) If $k = 2$, then G has $n+1$ edges and this implies that G is a connected bicyclic graph. Since the sum of the degrees of G equals $2n+2$ it follows that the degree sequence of G is $d_1(G) = [3^2, 2^{n-2}]$ or $d_2(G) = [4^1, 2^{n-1}]$. If the degree sequence is $d_1(G)$ then G consists of: a) two cycles having a common path of length $l \geq 1$, or b) two cycles joined by a path of length $l \geq 1$. If the degree sequence is $d_2(G)$ then G is composed of c) two cycles having a common vertex. In cases a) and b) if $l = 1$ then $\chi_\alpha(G) = (n-4)4^\alpha + 4 \cdot 5^\alpha + 6^\alpha = A$ and if $l \geq 2$ then $\chi_\alpha(G) = (n-5)4^\alpha + 6 \cdot 5^\alpha = B$ and in the case c) we get $\chi_\alpha(G) = (n-3)4^\alpha + 4 \cdot 6^\alpha = C$. We get $A > B$ since this inequality is equivalent to $4^\alpha + 6^\alpha > 2 \cdot 5^\alpha$. This can be deduced from Jensen's inequality written for the function x^α, which is strictly convex for $\alpha > 1$. Also $C > A$ holds since this inequality is equivalent to $4^\alpha + 3 \cdot 6^\alpha > 4 \cdot 5^\alpha$ and it can be deduced from the inequalities $4^\alpha + 6^\alpha > 2 \cdot 5^\alpha$ and $2 \cdot 6^\alpha > 2 \cdot 5^\alpha$.

The conclusion follows since for $n = 4$ the unique bicyclic graph is $K_4 - e$ for which $\chi_\alpha(K_4 - e) = 4 \cdot 5^\alpha + 6^\alpha$. The extremal graph is unique only for $n = 4$ and $n = 5$ since for $n = 6$ we have two extremal graphs: C_5 and C_4 with a common path P_3 and two cycles C_5 with a common path P_4.

3. Acknowledgments

This research is supported by the UPAR Grant of United Arab Emirates, Al-Ain, UAE via Grant No. G00002590.

REFERENCES

[1] *N. Akhter, M. K. Jamil, I. Tomescu*, Extremal first and second Zagreb indices of apex trees, U. P. B. Sci. Bull., Series A, **78(4)** (2016) 221-230.

[2] *A. Bondy, U.S.R. Murty*, Graph Theory with Applications, Macmillan Press Ltd., London, (1976).

[3] *I. Gutman, M. K. Jamil, N. Akhter*, Graphs with fixed number of pendent vertices and minimal first Zagreb index, Transactions on Combinatorics, **4**(1) (2015) 43-48.

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

[5] *Y. Hu, X. Li and Y. Yuan*, Trees with maximum general Randić indices, MATCH Commun. Math. Comput. Chem., **52** (2004) 129-146.

[6] *M. K. Jamil, I. Tomescu*, Zeroth-order general Randić index of k-generalized quasi trees, arXiv:1801.03885v1 [math.CO] 11 Jan 2018.

[7] *L. B. Kier, L.H. Hall*, Molecular Connectivity in Chemistry and Drug Research, Academic Press, New York, 1976.

[8] *L. B. Kier, L.H. Hall*, Molecular Connectivity in Structure-analysis, Research Studies Press, Wiley, Chichester, UK, 1986.

[9] *X. Li, H. Zhao*, Trees with the first three smallest and largest generalized topological indices, MATCH Commun. Math. Comp. Chem., **50** (2004) 57-62.

[10] *S. Qiao*, On zeroth-order general Randić index of quasi-tree graphs containing cycles, Discrete Optimization, **7** (2010) 93-98.

[11] *B. Zhou, N. Trinajstić*, On general sum-connectivity index, J Math Chem **47** (2010) 210-218.