

Proceedings of the 2nd International Conference on Combinatorics, Cryptography and Computation (I4C2017)

Sharp Bounds on First and Second Multiplicative Zagreb Indices for *t*-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. m.kamran.sms@gmail.com

Hafiz Mutee ur Rehman, Ali Raza Department of Mathematics & Statistics, The University of Lahore, Lahore, Pakistan. rehman.mutee@yahoo.com, ali_pu2002@yahoo.com

Asbtract

For a graph G, the first and second multiplicative Zagreb indices are defined as $\prod_1(G) = \prod_{v \in V(G)} d(v)^2$ and $\prod_2 = \prod_{uv \in E(G)} d(u)d(v)$, respectively, where d(v) is the degree of the vertex v in the graph G. Let $QT_t(n)$ be the set of t-generalized quasi-trees with n vertices. In this paper, we determined the extremal elements from the set $QT_t(n)$ with respect to the first and second multiplicative Zagreb indices.

keyword: t-generalized quasi trees, multiplicative Zagreb indices, degree of vertex, extremal graphs.

1. Introduction

Let G = (V(G), E(G)) be a graph, where V(G) is the set of vertices and E(G) represents the set of edges of the graph G. All graphs considered in this paper are finite, simple, connected and undirected. For notations and terminology not defined here see [3]. The degree of a vertex $v \in V(G)$ in a graph G is the number of vertices adjacent to the vertex v in G, it is denoted as d(v). The minimum degree in a graph G is denoted as $\delta(G)$. 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. Let V_t denotes the subset of vertex set V(G) with cardinality t in a graph G, then $G - V_t$ is the graph obtained from G by removing all the t vertices in the subset V_t and its incident edges.

In a graph G, if there exist a vertex $v \in V$ 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. Similarly, a graph G is called a t-generalized quasi tree, if there exist a subset $V_t \subset V(G)$ such that $G - V_t$ is a tree but for any other subset $V_{t-1} \subset V(G)$, $G - V_{t-1}$ is not a tree. The vertices in V_t are called the t-quasi vertices or simply quasi vertices. In a tree, deletion of any vertex with degree one will deduce another tree it follows that any tree is a quasi-tree. Trees are called trivial quasi-trees and other quasi-trees are called non-trivial quasi-trees. $QT_t(n)$ is the collection of nontrivial t-generalized quasi-trees with n vertices. The complete, path, star, double star graphs and tree with nvertices are denoted as K_n , P_n , S_n , $S_{p,q}$ (where p+q=n) and T_n , respectively.

Let G_1 and G_2 be two vertex disjoint graphs. $G_1 + G_2$ denoted the join graph of G_1 and G_2 with vertex set $V(G_1 + G_2) = V(G_1) \cup V(G_2)$ and the edge set $E(G_1 + G_2) = E(G_1) \cup E(G_2) \cup \{uv | u \in V(G_1), v \in V(G_2)\}$. Let $u, v \in V(G_2), G_1 \bullet_{u,v} G_2$ represents the graph having vertex set $V(G_1) \cup V(G_2)$ and obtained by joining every vertex of G_1 to vertices u and v of G_2 .

In 1972, Gutman and Trinajstič [8] introduced the oldest degree based topological indices under the name first and second Zagreb index and defined

as

$$M_1(G) = \sum_{v \in V(G)} d(v)^2$$
$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

In 2010, Todeschini and Consonni [12] proposed the multiplicative versions of Zagreb indices. The first and second multiplicative Zagreb indices of a graph G are defined as

$$\prod_{1} (G) = \prod_{v \in V(G)} d(v)^{2}$$
$$\prod_{2} (G) = \prod_{uv \in E(G)} d(u)d(v) = \prod_{v \in V(G)} d(v)^{d(v)}$$

For history, mathematical properties and applications of the Zagreb indices we refer [2, 4, 6, 7, 9, 11, 13, 14].

In [1] and [10] Jamil et. al. determined the bounds on first and second Zagreb and Zeroth-order general Randic index for t-generalized quasi-trees, respectively. In this paper, we investigated the bounds on multiplicative Zagreb indices and characterized the extremal graphs.

2. Main Results

In this section, first we will discuss some preliminaries lemmas which will be useful in later to prove our main theorems.

By definition of first and second Multiplicative Zagreb indices we have the following result.

Lemma 1. Let $u, v \in V(G)$ such that $uv \notin E(G)$, then

$$\prod_{i} (G+uv) > \prod_{i} (G), i = 1, 2$$
$$\prod_{i} (G-uv) < \prod_{i} (G), i = 1, 2$$

Lemma 2. Let n,m,r and x_i , where $1 \le i \le n$, are positive integers such that $x_1 + x_2 + \cdots + x_n = r$.

i) The function $f(x_1, x_2, \dots, x_n; r) = \prod_{i=1}^n x_i^2$ is maximum if and only if x_1, x_2, \dots, x_n are almost equal, i.e. $|x_i - x_j| \leq 1$ for every $1 \leq i, j \leq n$. ii) If $x_1 \geq x_2 \geq m$, the minimum of the function $f(x_1, \dots, x_n; r)$ reached only when $x_1 = r - m - n + 2$, $x_2 = m$ and $x_j = 1$ for $3 \leq j \leq n$. The second minimum is reached only for $x_1 = r - m - n + 1$, $x_2 = m + 1$ and $x_j = 1$ for $3 \leq j \leq n$.

PROOF. i) For x > 0, $g(x) = \frac{x^2}{(x+1)^2}$ is a strictly increasing function. If $x \ge y+2 > 0$ we deduce x-1 > y, this implies g(x-1) > g(y), or $x^2y^2 < (x-1)^2(y+1)^2$. It follows that $f(x_1, x_2, \dots, x_n; r) = \prod_{i=1}^n x_i^2$ is maximum if and only if x_1, x_2, \dots, x_n are almost equal.

ii) If $x \ge y \ge 2$ then x > y - 1, then g(x) > g(y - 1) this implies that $x^2y^2 > (x + 1)^2(y - 1)^2$.

Lemma 3. Let n,m,r and x_i , where $1 \le i \le n$, are positive integers such that $x_1 + x_2 + \cdots + x_n = r$.

i) The function $f(x_1, x_2, \dots, x_n; r) = \prod_{i=1}^n x_i^{x_i}$ is minimum if and only if x_1, x_2, \dots, x_n are almost equal, i.e. $|x_i - x_j| \leq 1$ for every $1 \leq i, j \leq n$. ii) If $x_1 \geq x_2 \geq m$, the maximum of the function $f(x_1, \dots, x_n; r)$ reached only for $x_1 = r - m - n + 2, x_2 = m + 1$ and $x_j = 1$ for $3 \leq j \leq n$.

PROOF. i) For x > 0, $h(x) = \frac{x^x}{(x+1)^{(x+1)}}$ is a strictly decreasing function. If $x \ge y+2 > 0$ we deduce x-1 > y, this implies h(x-1) < h(y), or $x^x y^y < (x-1)^{(x-1)} (y+1)^{(y+1)}$. It follows that $f(x_1, x_2, \dots, x_n; r) = \prod_{i=1}^n x_i^{(x_i)}$ is minimum if and only if x_1, x_2, \dots, x_n are almost equal. ii) If $x \ge y \ge 2$ then x > y - 1, then h(x) < g(y-1) this implies that

 $x^{x}y^{y} < (x+1)^{(x+1)}(y-1)^{(y-1)}.$

Lemma 4. Let $QT_t(n)$. If $\prod_i(G)$, i=1,2, is minimum then there exists a spanning subgraphs K of G such that $\prod_i(G) \ge \prod_i(K)$ and for any quasi vertex z of G we have $d_G(z) \ge d_K(z)=2$ and z is adjacent in K to at least two other vertices in G - X, where x is the set of quasi vertices.

PROOF. By definition of a *t*-generalized quasi tree, there exists a subset $V_t(G) \subset V(G)$ such that $G - V_t$ is a tree and for any $V_{t-1} \subset V(G)$, $G - V_{t-1}$ is not a tree. It follows that $d(z) \geq 2$ for any vertex $z \in V_t(G)$. If *m* denotes

the number of edges of G, then $m \ge 2t + n - t - 1 = n + t - 1$ and equality holds if and only if d(z) = 2 for any vertex $z \in V_t$ and no two vertices in V_t are adjacent. By Lemma 1, by deleting some edges it follows the existence of the graph K, which is not necessarily in $QT_t(n)$.

Lemma 5. Let $G \in QT_t(n)$, where $n \ge 3, t \ge 1$ and $\prod_i(G)$ (i=1,2) is as large as possible and z is a quasi vertex of G then, d(z)=n-1.

PROOF. Let $G \in QT_t(n)$, $\prod_i(G)$ is as large as possible 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 $QT_t(n)$ and $\prod_i(G + xz) > \prod_i(G)$, a contradiction, hence d(z) = n - 1.

Lemma 6. Let G be a graph and u,w and x be three vertices of G such that d(u) < d(w), $xw \notin E(G)$ and $xu \in E(G)$. If we obtained a graph G' = G - xu + xw then

$$\prod_1(G') < \prod_1(G)$$

PROOF. By the definition of first multiplicative Zagreb index

$$\begin{split} \prod_{1} (G') &- \prod_{1} (G) = \prod_{\substack{v \in V(G) \\ v \neq u, u \neq w}} d(v)^{2} \Big[(d(u) - 1)^{2} (d(w) + 1)^{2} - d(u)^{2} d(w)^{2} \Big] \\ &= \prod_{\substack{v \in V(G) \\ v \neq u, u \neq w}} d(v)^{2} \Big(d(u) - d(w) - 1 \Big) \Big(2d(u)d(w) + d(u) - d(w) - 1 \Big) \\ &< 0 \end{split}$$

Theorem 7. Let $G \in QT_t(n)$, where $n \ge 3$ and $t \ge 1$ then

$$\prod_{1} (G) \le (n-1)^{2t} (t+1)^4 (t+2)^{2(n-t-2)}$$

equality holds if and only if $G = K_t + P_{n-t}$.

PROOF. Let $G \in QT_t(n)$ has the maximum $\prod_1(G)$. Let $V_t \subset V(G)$ be the set of t quasi vertices. As $\prod_1(G + uv) > \prod_1(G)$ for any $uv \notin E(G)$ this implies that V_t forms a complete graph. Then by Lemma 5 we have $G = K_t + T_{n-t}$.

$$\prod_{1} (G) = \prod_{1} (K_t + T_{n-t})$$

=
$$\prod_{v \in V(K_t)} (d(v) + n - t)^2 \cdot \prod_{v \in V(T_{n-t})} (d(v) + t)^2$$

=
$$(n - 1)^{2t} \cdot \prod_{v \in V(T_{n-t})} (d(v) + t)^2$$

By Lemma 2, $\prod_{v \in V(T_{n-t})} (d(v) + t)^2$ is maximum if and only if the degrees of T_{n-t} are almost equal i.e. $T_{n-t} = P_{n-t}$. So we obtained

$$\prod_{v \in V(T_{n-t})} (d(v) + t)^2 = (t+1)^4 (t+2)^{2(n-t-2)}$$

Hence the right hand inequality

$$\prod_{1} (G) \le (n-1)^{2t} (t+1)^4 (t+2)^{2(n-t-2)}$$

and the equality holds if and only if $G = K_t + P_{n-t}$.

Theorem 8. Let $G \in QT_t(n)$, where $n \ge 3$ and $t \ge 1$. We have *i*) If t = 1 then

$$(n-1)^2(t+1)^2 4^t \le \prod_1 (G)$$

equality holds if and only if $\overline{K_t} \bullet_{u,v} S_{n-1}$, where u is the center of S_{n-1} and v is a pendant vertex of S_{n-1} . ii) If $n \ge 4$ and $t \ge 2$ then

$$(n-2)^2(t+2)^2 4^t \le \prod_1 (G)$$

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

PROOF. Let $G \in QT_t(n)$ has the minimum $\prod_1(G)$. Let $V_t \subset V(G)$ be the set of t quasi vertices. As, $\prod_1(G - uv) < \prod_1(G)$ for any $uv \in E(G)$ this implies that V_t forms an empty graph, i.e. $\overline{K_t}$. But by Lemma 4 every quasi vertex has degree 2 and by Lemma 6 quasi vertices must have common neighbors $y_1, y_2 \notin V_t(G)$, since G is minimum. We represent the graph G as $G = \overline{K_t} \bullet_{y_1,y_2} T_{n-t}$

$$\prod_{1} (\overline{K_t} \bullet T_{n-t}) = \prod_{v \in V(\overline{K_t} \bullet T_{n-t})} d(v)^2$$
$$= \prod_{v \in V(\overline{K_t})} d(v)^2 \cdot \prod_{\substack{v \in V(T_{n-t}) \\ v \neq y_1, v \neq y_2}} d(v)^2 \cdot (d(y_1) + t)^2 \cdot (d(y_2) + t)^2$$

By Lemma 2, the product

$$\prod_{\substack{v \in V(T_{n-t})\\v \neq y_1, v \neq y_2}} d(v)^2 \cdot (d(y_1) + t)^2 \cdot (d(y_2) + t)^2 \tag{1}$$

is minimum only if $T_{n-t} = S_{n-t}$ and y_1 and y_2 are the center and a pendent vertex of S_{n-t} . For t = 1, this graph is a t-generalized quasi-tree, but for $t \ge 2$ this property is no longer valid. We must consider the second minimum of Eq. 1. This time $H \in QT_t(n)$, G = H and $T_{n-t} = S_{n-t-2,2}(u, v)$, $y_1 = u$ and $y_2 = v$. Hence the result.

Theorem 9. Let $G \in QT_t(n)$, where $n \ge 3$ and $t \ge 1$ then

$$\prod_{2} (G) \le (n-1)^{(n-1)(t+1)} (t+1)^{(t+1)(n-t-1)}$$

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

PROOF. Let $G \in QT_t(n)$ has the maximum $\prod_2(G)$. Let $V_t \subset V(G)$ be the set of t-quasi vertices. As $\prod_2(G + uv) > \prod_2(G)$ for any $uv \notin E(G)$ this implies that V_t forms a complete graph. Then by Lemma 5 we have $G = K_t + T_{n-t}$.

$$\prod_{2} (G) = \prod_{2} (K_t + T_{n-t})$$

=
$$\prod_{v \in V(K_t)} (d(v) + n - t)^{d(v)} \cdot \prod_{v \in V(T_{n-t})} (d(v) + t)^{d(v)}$$

=
$$(n-1)^{(n-1)t} \cdot \prod_{v \in V(T_{n-t})} (d(v) + t)^{d(v)}$$

By Lemma 3, the product

$$\prod_{v \in V(T_{n-t})} (d(v) + t)^{d(v)}$$

is maximum only if $T_{n-t} = S_{n-t}$. Hence, we obtained

$$\prod_{2} (G) \le (n-1)^{(n-1)(t+1)} (t+1)^{(t+1)(n-t-1)}$$

equality holds if and only if $G = K_t + S_{n-t}$

Theorem 10. Let $G \in QT_t(n)$, where $n \ge 3$ and $t \ge 1$ then

$$\prod_{2} (G) \ge 2^{2(n-2t-2)} \cdot 3^{6(t-1)}$$

equality holds if and only if G has n-2t+2 vertices of degree 2 and 2t-2 vertices of degree 3..

PROOF. Suppose that $\prod_2(G)$ is minimum. By Lemma 4 there exists a spanning subgraph K of G such that $\prod_2(G) \ge \prod_2(K)$ and every quasi vertex z has $d_K(z) = 2$, which implies that $\sum_{v \in V(G)} d_K(v) = 2(n+t-1)$. By Lemma 3 $\prod_2(K)$ is minimum if the degrees of K are almost equal to 2 or 3. Let n_i is the number of vertices having degree i we can write $2n_2+3(n-n_2) = 2n+2t-2$, which implies $n_2 = n - 2t + 2$ and $n_3 = n - n_2 = 2t - 2$. Consequently, the minimum of $\prod_2(G)$ is reached if and only if there exist n - 2t + 2 vertices (including quasi vertices) of degree 2 and 2t - 2 vertices of degree 3 (in this case K = G). Such a graph is depicted in Fig. 1.



Figure 1: An example of *t*-generalized quasi-tree with almost equal degree vertices.

References

- 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] J. Braun, A. Kerber, M. Meringer, C. Rucker, Similarity of molecular descriptors: The equivalence of Zagreb indices and walk counts, MATCH Commun. Math. Comput. Chem. 54 (2005) 163-176.
- [3] A. Bondy, U. S. R. Murty, Graph theory with applications, Macmillan Press Ltd., London, (1976).
- [4] M. Eliasi, I. Gutman, A. Iranmanesh, Multiplicative Versions of first Zagreb index, MATCH Commun. Math. Comput. Chem. 68 (2012) 217230.
- [5] I. Gutman, Multiplicative Zagreb indices of trees, Bulletin of International Mathematical Virtual Institute, 1(2011), 13-19.
- [6] I. Gutman, Multiplicative Zagreb indices of trees, Bull. Int. Math. Virt. Inst. 1 (2011) 1319.
- [7] I. Gutman, K. C. Das, The first Zagreb index 30 years after, MATCH Commun. Math. Comput. Chem. 50 (2004) 83-92.
- [8] I. Gutman, N. Trinajstič, Graph theory and molecular orbitals. Total π electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972) 535-538.
- [9] I. Gutman, M. K. Jamil, N. Akhter, Graphs with fixed number of pendent vertices and minimal first Zagreb index, 4(1) (2015) 43-48.
- [10] M. K. Jamil, I. Tomescu, Zeroth-order general Randic index of kgeneralized quais trees, preprint.
- [11] S. Nikolić, G. Kovačević, A. Milicević, N. Trinajstić, The Zagreb indices 30 years after, Croat. Chem. Acta 76 (2003) 113124.
- [12] R. Todeschini, D. Ballabio, V. Consonni, Novel molecular descriptors based on functions of new vertex degrees. In: Novel molecular structure descriptors Theory and applications I. (I. Gutman, B. Furtula, eds.), Kragujevac: Univ. Kragujevac (2010) 73-100.

- [13] D. Vukičević, I. Gutman, B. Furtula, V. Andova, D. Dimitrov, Some observations on comparing Zagreb indices, MATCH Commun. Math. Comput. Chem. 66 (2011) 627-645.
- [14] B. Zhou, Zagreb indices, MATCH Commun. Math. Comput. Chem. 52 (2004) 113- 118.