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Generalized Schultz and Gutman Indices

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ABSTRACT

The degree and distance both are significant concepts in graphs with wide spread utilization. The combined study of these concepts has given a new direction to the topological indices. In this article, we present the generalized degree distance indices (Generalized First Schultz indices) $DD(a,b)$ and generalized Gutman indices (Second Schultz indices) $ZZ(a,b)$. The computed values of these indices on certain families of graphs along with some bounds and characterizations are obtained. Also, we present the relationship between $DD(a,b)$ and $ZZ(a,b)$. Further, we present the Schultz polynomials along with the statistical analysis of certain graphs.

1. INTRODUCTION

The graph $G = (V,E)$, which is discussed in this paper is finite, undirected graph, without loops or multiple edges. In general, we use, $p = |V|$ and $q = |E|$ to denote the number of vertices and edges of a graph G, respectively. The number of edges adjacent to a vertex called the degree of a vertex; the minimum degree is denoted by $\delta(G)$ and the maximum

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degree is denoted by $\Delta(G)$. For graph-theoretical terminology and notation not defined here we follow [2], [7] and [18].

The degree distance indices (First Schultz indices) and Gutman indices (Second Schultz indices) are well known. The Schultz index was introduced by Harry P. Schultz [13] in 1989 defined as molecular topological index $MTI(G) = \sum_{i=1}^{p}|v(A+D)|$, where A and $D = \|d(u_i,u_j)\|$ are the adjacency and distance matrices of G and $v = (\mathrm{d}(v_1), \mathrm{d}(v_2),\ldots,\mathrm{d}(v_p))$, respectively, see [5]. Dobrynin et al. [5] and Gutman [9] separately studied the weighted version of Wiener index and the Gutman indices. Here, we study the generalized version of the first and second Schultz indices. For more details, we refer to [1, 3, 4, 6, 8, 10, 11, 12, 14, 15, 16, 17] and [18].

2. THE FIRST GENERALIZED SCHULTZ INDEX

For any positive real values a and b, the generalized first Schultz index is given by

$$DD_{(a,b)}(G) = \sum_{\{u_i,u_j\}\subseteq V(G)}(d(u_i)+d(u_j))^a(d(u_i,u_j))^b.$$

Here, we obtained bounds of $DD_{(a,b)}(G)$ in terms of order p, size q, maximum degree $\Delta(G)$, minimum degree $\delta(G)$, distance $d(u_i,u_j)$ and radius $rad(G)$.

Theorem 2.1. *For any connected graph G with radius $rad(G)$,*

$$\frac{p(p-1)}{2}[\delta(G)]^{2a}[rad(G)]^b \le DD_{(a,b)}(G) \le \frac{p(p-1)}{2}[\Delta(G)]^{2a}[rad(G)]^b.$$

Proof. Let G be a connected graph with $p \ge 3$. We know that

$$\delta(G) \le d(u_i) + d(u_j) \le \Delta(G). \tag{1}$$

$$(\delta(G))^{2a} \le \left(d(u_i)+d(u_j)\right)^a \le \left(\Delta(G)\right)^{2a}. \tag{2}$$

$$rad(G) \le d(u_i,u_j) \le 2rad(G). \tag{3}$$

$$(rad(G))^b \le (d(u_i,u_j))^b \le (2rad(G))^b. \tag{4}$$

Multiplying equations (2) and (4), we have

$$[\delta(G)]^{2a}[rad(G)]^b \le (d(u_i)+d(u_j))^a(d(u_i,u_j))^b \le [\Delta(G)]^{2a}[rad(G)]^b$$

$$\frac{p(p-1)}{2}[\delta(G)]^{2a}[rad(G)]^b \le DD_{(a,b)}(G) \le \frac{p(p-1)}{2}[\Delta(G)]^{2a}[rad(G)]^b.$$

■

Theorem 2.2. *For any connected graph G with $p \ge 3$,*

$$\frac{p(p-1)}{2}2^a[rad(G)]^b \le DD_{(a,b)}(G) \le \frac{p}{2}2^a(p-1)^{a+1}[2rad(G)]^b.$$

Proof. Let G be a connected graph with $p \geq 3$. We know that

$$1 \leq d(u_i) \leq p-1. \tag{5}$$

$$2 \leq d(u_i) + d(u_j) \leq 2(\mathrm{p}-1). \tag{6}$$

$$2^a \leq (d(u_i) + d(u_j))^a \leq (2(\mathrm{p}-1))^a. \tag{7}$$

$$(rad(G))^b \leq (d(u_i, u_j))^b \leq (2\, rad(G))^b. \tag{8}$$

Multiplying equations (7) and (8), we have

$$2^a[rad(G)]^b \leq (d(u_i) + d(u_j))^a (d(u_i, u_j))^b \leq [2(\mathrm{p}-1)]^a [rad(G)]^b.$$

$$\tfrac{p(p-1)}{2} 2^a [rad(G)]^b \leq DD_{(a,b)}(G) \leq \tfrac{p}{2} 2^a [(\mathrm{p}-1)]^{a+1} [2rad(G)]^b.$$ ∎

Theorem 2.3. *Let G be any connected graph with $p \geq 3$. Then,*

$$\tfrac{p(p-1)}{2} 2^a \leq DD_{(a,b)}(G) \leq \tfrac{p}{2} 2^a (p-1)^{a+b+1}.$$

Proof. Let G be a connected graph with $p \geq 3$. We know that

$$2^a \leq (d(u_i) + d(u_j))^a \leq (2(\mathrm{p}-1))^a. \tag{9}$$

$$1 \leq d(u_i, u_j) \leq p-1. \tag{10}$$

$$1 \leq (d(u_i, u_j))^b \leq (p-1)^b. \tag{11}$$

Multiplying equations (9) and (11), we have

$$2^a \leq (d(u_i) + d(u_j))^a (d(u_i, u_j))^b \leq [2(\mathrm{p}-1)]^a (p-1)^b.$$

$$\frac{p(p-1)}{2} 2^a \leq DD_{(a,b)}(G) \leq \frac{p(p-1)}{2} [2(\mathrm{p}-1)]^a (p-1)^b.$$

$$\tfrac{p(p-1)}{2} 2^a \leq DD_{(a,b)}(G) \leq \tfrac{p}{2} 2^a (p-1)^{a+b+1}.$$ ∎

Theorem 2.4. *For any connected graph G with $p \geq 3$,*

$$\tfrac{p(p-1)}{2} (2\delta(G))^a \leq DD_{(a,b)}(G) \leq \tfrac{p}{2} (2\Delta(G))^a (p-1)^{b+1}.$$

Proof. Let G be a connected graph with $p \geq 3$. We know that

$$(2\delta(G))^a \leq (d(u_i) + d(u_j))^a \leq (2\Delta(G))^a. \tag{12}$$

$$1 \leq d(u_i, u_j) \leq p-1. \tag{13}$$

$$1 \leq (d(u_i, u_j))^b \leq (p-1)^b. \tag{14}$$

Multiplying equations (12) and (14), we have

$$\tfrac{p(p-1)}{2} (2\delta(G))^a \leq DD_{(a,b)}(G) \leq \tfrac{p}{2} (2\Delta(G))^a (p-1)^{b+1}.$$ ∎

Theorem 2.5. *Let G be any connected graph with $p \geq 3$ vertices. Then,*

$$(4q(p-1) - M_1(G))^a + \left(2\delta(G)\right)^a \left(2W(G) + q - p(p-1)\right)^b \leq DD_{(a,b)}(G)$$
$$\leq (4q(p-1) - M_1(G))^a + \left(2\Delta(G)\right)^a \left(2W(G) + q - p(p-1)\right)^b.$$

Proof. Let G be a connected graph with $p \geq 3$. Then, we prove the upper bound,

$$
\begin{aligned}
DD_{(a,b)}(G) &= \sum_{u_i \in V(G)} d(u_i)^a D(u_i)^b = \sum_{u_i \in V(G)} d(u_i)^a \sum_{u_i \in V(G)} D(u_i)^b \\
&= \sum_{\{u_i,u_j\} \subseteq V(G)} (d(u_i) + d(u_j))^a (d(u_i,u_j))^b \\
&= \sum_{u_i,u_j \in E(G)} (d(u_i) + d(u_j))^a + \sum_{\{u_i,u_j\} \subseteq V(G);\, d(u_i,u_j) \geq 2} 2(d(u_i) + d(u_j))^a \\
&\quad + \sum_{\{u_i,u_j\} \subseteq V(G);\, d(u_i,u_j) \geq 2} (d(u_i) + d(u_j))^a (d(u_i,u_j) - 2)^b \\
&\leq \sum_{i=1}^{p} (d(u_i))^{2a} + \sum_{i=1}^{p} (d(u_i)(p - d(u_i) - 1) + (2q - d(u_i) - d(u_i)\mu_i))^a \\
&\quad + \sum_{1 \leq i \leq j \leq p;\, d(u_i,u_j) \geq 2} (d(u_i) + d(u_j))^a (d(u_i,u_j) - 2)^b.
\end{aligned}
$$

Since, we have $(2\delta)^a \leq \sum \left(d(u_i) + d(u_j)\right)^a \leq (2\Delta)^a$

where $d(u_i)\mu_i = \sum_{u_i,u_j \in E(G)} d(u_j)$

$$
\begin{aligned}
&\leq (4q(p-1) - M_1(G))^a \\
&\quad + (2\Delta(G))^a \left(\sum_{u_i,u_j \in V(G);\, d(u_i,u_j) \geq 2} (d(u_i,u_j) - 2 \sum_{u_i,u_j \in V(G);\, d(u_i,u_j) \geq 2} 1\right)^b,
\end{aligned}
$$

where $M_1(G) = \sum_{i=1}^{p} (d(u_i))^2 = \sum_{i=1}^{p} d(u_i)\mu_i$

$$
\leq (4q(p-1) - M_1(G))^a + (2\Delta(G))^a (2W(G) + q - p(p-1))^b.
$$

To prove the lower bound we have

$$
\begin{aligned}
DD_{(a,b)}(G) &= \sum_{u_i \in V(G)} d(u_i)^a D(u_i)^b = \sum_{u_i \in V(G)} d(u_i)^a \sum_{u_i \in V(G)} D(u_i)^b \\
&= \sum_{\{u_i,u_j\} \subseteq V(G)} (d(u_i) + d(u_j))^a (d(u_i,u_j))^b \\
&= \sum_{u_i,u_j \in E(G)} (d(u_i) + d(u_j))^a + \sum_{\{u_i,u_j\} \subseteq V(G);\, d(u_i,u_j) \geq 2} 2(d(u_i) + d(u_j))^a \\
&\quad + \sum_{\{u_i,u_j\} \subseteq V(G);\, d(u_i,u_j) \geq 2} (d(u_i) + d(u_j))^a (d(u_i,u_j) - 2)^b \\
&\geq \sum_{i=1}^{p} (d(u_i))^{2a} + \sum_{i=1}^{p} (d(u_i)(p - d(u_i) - 1) + (2q - d(u_i) - d(u_i)\mu_i))^a \\
&\quad + \sum_{1 \leq i \leq j \leq p;\, d(u_i,u_j) \geq 2} (d(u_i) + d(u_j))^a (d(u_i,u_j) - 2)^b.
\end{aligned}
$$

Since, we have $(2\delta)^a \leq \sum (d(u_i) + d(u_j))^a \leq (2\Delta)^a$

where $d(u_i)\mu_i = \sum_{u_i,u_j \in E(G)} d(u_j)$
$\geq (4q(p-1) - M_1(G))^a$
$+(2\delta(G))^a \ \left(\sum_{u_i,u_j \in V(G);\, d(u_i,u_j)\geq 2} (d(u_i,u_j) - 2\sum_{u_i,u_j \in V(G);\, d(u_i,u_j)\geq 2} 1\right)^b,$
where $M_1(G) = \sum_{i=1}^{p}(d(u_i))^2 = \sum_{i=1}^{p} d(u_i)\mu_i$
$\geq (4q(p-1) - M_1(G))^a + (2\delta(G))^a(2W(G) + q - p(p-1))^b.$

■

Proposition 2.1. *Let G be the class of some standard graphs. Then,*

(i) $DD_{(a,b)}(C_p) = \begin{cases} 2p(4)^a\left(\frac{(p^2-1)}{8}\right)^b & if\ p\ is\ odd \\ 2p(4)^a\left(\frac{(p-1)^2-1}{8}\right)^b + p(4)^a\left(\frac{p}{8}\right)^b & if\ p\ is\ even \end{cases}.$

(ii) $DD_{(a,b)}(K_p) = p2^a(p-1)^{a+1}.$

(iii) $DD_{(a,b)}(K_{1,p-1}) = (p-1)((p-2)2^{a+b} + 2p^a).$

(iv) $DD_{(a,b)}(W_p) = 2(p-1)((p+2)^a) + 6^a + (p-4)6^a2^{b-1}.$

Proof. Let C_p be a cycle with $p \geq 3$. Then the degree of each vertex is $d(u) = 2$ and the maximum distance that exists is $\left\lfloor\frac{p}{2}\right\rfloor$. Therefore,

Case 1. If p is odd, then there exists a p-number of degree partitions for all the distance. This implies that $p\{d(u) + d(v)\}\left\{1 + 2 + \cdots + \left\lfloor\frac{p}{2}\right\rfloor\right\}$. Therefore $DD_{(a,b)}(C_p) = p(4^a)\left(\frac{(p^2-1)^b}{8}\right)$ follows.

Case 2. If p is even, then there exists a p-number of degree partitions for the distances up to $\frac{(p-2)}{2}$ and $\frac{p}{2}$-number of degree sum partitions for the distance. This is equivalent to $p\{d(u) + d(v)\}\left\{1 + 2 + \cdots + \frac{(p-2)}{2}\right\} + \frac{p}{2}\{d(u) + d(v)\}\frac{p}{2}$. Therefore

$$DD_{(a,b)}(C_p) = p(4^a)\left(\frac{(p^2-1)^2-1}{8}\right)^b + 4^a\left(\frac{p}{2}\right)^{b+1}.$$

Let K_p be a complete graph with $p \geq 3$ vertices. Then the degree of each vertex is $d(u) = (p-1)$ and only one distance exists. Thus, there are $\frac{p(p-1)}{2}$-number of degree partitions occur for the distance. This implies that $\frac{p(p-1)}{2}[d(u) + d(v)]$ and hence

$$DD_{(a,b)}(K_p) = \frac{p(p-1)}{2}[(p-1)+(p-1)]^a 1^b = p2^{a-1}(p-1)^{a+1}.$$

Let $K_{1,p-1}$ be a star with $p \geq 3$ vertices. Then there exists a $(p-1)$ – number of degree partition $(1, p-1)$ for the distance one and $\frac{(p-1)(p-2)}{2}$ – number of degree partition (1,1) for the distance two. This implies that

$$DD_{(a,b)}(K_{1.p-1}) = (p-1)(1+p-1)^a + \frac{(p-1)(p-2)}{2}(1+1)^a 2^b$$

$$= (p-1)p^a + (p-1)(p-2)2^{a+b-1}.$$

Let W_p be a wheel with $p \geq 4$ vertices. Then the degree of the surrounded vertices are three and centre vertex is $(p-1)$ and maximum distance that exists is two. For the distance one, there are $(p-1)$-number of surrounded degree partitions and $(p-1)$-number of surrounded degrees with centre vertex degree. For the distance two, there are $\frac{(p-1)(p-4)}{2}$-number of surrounded degree partitions. This implies that

$$DD_{(a,b)}(W_p) = (p-1)(3+3)^a + (p-1)(3+p-1)^a$$

$$+\frac{(p-1)(p-4)}{2}(3+3)^a 2^b$$

$$= (p-1)[6^a + (p+2)^a + (p-4)6^a 2^{b-1}. \quad \blacksquare$$

The corona $G_1 \circ G_2$ is the graph obtained from the graphs G_1 and G_2 by taking one copy of G_1 and $|V(G_1)|$ copies of G_2 and then joining each vertex of the i^{th} copy of G_2 named (G_2, i), with the i^{th} vertex of G_1 by an edge.

Theorem 2.6. *Let* $G \cong C_{p1} \circ K_{p2}$ *with* $p_1 \geq 3$ *and* $p_2 \geq 1$. *Then,*

$$DD_{(a,b)}(G) = \begin{cases} p_1p_2(2p_2)^a\left(\frac{p_1}{2}+2\right)^b + p_1(2p_2+4)^a\left(\frac{p_1}{2}+1\right)^b & if\ p_2\ is\ odd \\ p_1p_2(2p_2)^a\left(\frac{p_1+2}{2}\right)^b + p_1(2p_2+4)^a\left(\frac{p_1+1}{2}\right)^b & if\ p_2\ is\ even \end{cases}.$$

Proof. Let $G \cong C_{p1} \circ K_{p2}$ with $p_1 \geq 3$ and $p_2 \geq 1$. Then, $d(u_i) = p_2 + 2$ for each vertex u_i of cycle C_{p1} and $d(u_j) = p_2$ for each vertex u_j of complete graph K_{p2}.

Case 1. For p_2 is odd, $d(u_i) = \frac{p_1}{2} + 1$ for each vertex u_i of cycle C_{p1} and $d(u_j) = \frac{p_1}{2} + 2$ for each vertex u_j of complete graph K_{p2}. Then,

$$DD_{(a,b)}(G) = \sum_{u_i,u_j \in V(G)} (d(u_i) + d(u_j))^a (d(u_i, u_j))^b$$
$$= p_1p_2(2p_2)^a \left(\frac{p_1}{2} + 2\right)^b + p_1(2(p_2 + 2))^a \left(\frac{p_1}{2} + 1\right)^b$$
$$= p_1p_2(2p_2)^a \left(\frac{p_1}{2} + 2\right)^b + p_1(2p_2 + 4)^a \left(\frac{p_1+2}{2}\right)^b.$$

Case 2. For p_2 is odd, $d(u_i) = \frac{p_1-1}{2} + 1$ for each vertex u_i of cycle C_{p1} and $d(u_j) = \frac{p_1-1}{2} + 2$ for each vertex u_j of complete graph K_{p2}. Then,

$$DD_{(a,b)}(G) = \sum_{u_i,u_j \in V(G)} (d(u_i) + d(u_j))^a (d(u_i, u_j))^b$$
$$= p_1p_2(2p_2)^a \left(\frac{p_1-2}{2} + 2\right)^b + p_1(2(p_2 + 2))^a \left(\frac{p_1-1}{2} + 1\right)^b$$
$$= p_1p_2(2p_2)^a \left(\frac{p_1+2}{2}\right)^b + p_1(2p_2 + 4)^a \left(\frac{p_1+1}{2}\right)^b.$$

■

2.1 HARARY GRAPH

In 1962, Harary introduced the Harary graph, an $n-$connected graph with p vertices of degree at least n and $\left\lceil\frac{np}{2}\right\rceil$ edges. The construction of $H_{n,p}$ depends on the relationship between n and p. Harary graph $H_{n,p}$ with $1 < n < p$ is constructed by placing equally spaced p vertices on a circle and joining them as follows:

Case 1. $n = 2m$ is even. By joining each vertex to its $\frac{n}{2}$ neighbors in each directions around the circle $H_{n,p}$ can be formed. Therefore, vertices $\left\{i, i+1, \dots, i+\frac{n}{2}\right\}$ and $\left\{i, i-1, \dots, i-\frac{n}{2}\right\}$ form clique in both the directions.

Case 2. n is odd and p is even. Let $n = 2m + 1$. Then $H_{n,p}$ is constructed by first drawing $H_{2m,p}$ and then adding edges joining the vertices i to $i + \frac{p}{2}; 1 \le i \le \frac{p}{2}$. Therefore, vertices between i to $i + \frac{n}{2}$ form a clique.

Case 3. n and p both are odd. Let $n = 2m + 1$. Then $H_{n,p}$ is constructed by first drawing $H_{2m,p}$ and then adding edges joining vertex 0 to vertices $\frac{p-1}{2}$ and $\frac{p+1}{2}$, and vertex i to $i + \frac{p+1}{2}; 1 \le i \le \frac{p}{2}$. Therefore, the degree of 0 is $n + 1$ while the degree of other vertices is n. For more details, see [15].

The Harary graphs and their matrices have important applications to the theory of designs and error-correcting codes. They are also, used as models for interconnection networks in telecommunication, VLSI designs, parallel, and distributed computing.

Theorem 2.7. *Let* $G \cong H_{n,p}$ *be a Harary graph with* $n \geq 2m; m \geq 1$ *and* $p \geq 4$ *and is even. Then,*

(i) $DD_{(a,b)}(G) = 2p(4)^a \left(\frac{(p-1)^2-1}{8}\right)^b + p(4)^a \left(\frac{p}{8}\right)^b$, if $m = 1$.

(ii) $DD_{(a,b)}(G) = np(2n)^a + p(p-n-1)(2n)^a(2)^b$, if $n = 2m$; $m \geq 2$.

Proof. Let $G \cong H_{n,p}$ be a Harary graph with $n \geq 2m; m \geq 1$ and $p \geq 4$ and is even. Then,

(i) If $m = 1$, the Harary graph is a cycle and it is a 2-regular graph. The maximum distance of the graph is $\left\lfloor \frac{p}{2} \right\rfloor$. The degree sequence will be $(2, 2, \dots, 2)$ and the distance sequence will be $\left(1, 2, \dots, \left\lfloor \frac{p}{2} \right\rfloor\right)$. Then the degree distance sequence will be $2p(2+2)\big(1+2+\cdots+(p-1)\big) + p(2+2)\frac{p}{2}$. Therefore,
$$DD_{(a,b)}(G) = 2p(4)^a \left(\frac{(p-1)^2-1}{8}\right)^b + p(4)^a \left(\frac{p}{8}\right)^b.$$

(ii) If $n = 2m$; $m \geq 2$, the graph is $r-$regular and p times of $(p-n-1)$ vertices are at the maximum distance at 2 and all other vertices at the distance 1. Then,
$$DD_{(a,b)}(G) = np(2n)^a + p(p-n-1)(2n)^a(2)^b.$$

■

Theorem 2.8. *Let* $G \cong H_{n,p}$ *be a Harary graph with* $n \geq 2m+1; m \geq 1$ *and* $p \geq 5$ *and is odd. Then,*
$$DD_{(a,b)}(G) = np(2n)^a + p(p-n-1)(2n)^a(2)^b.$$

Proof. Let $G \cong H_{n,p}$ be a Harary graph with $n \geq 2m+1$; $m \geq 1$ and $p \geq 5$ and is odd. Then, the graph is $r-$regular and p times of $(p-k-1)$ vertices have the distance 2 and the remaining vertices have distance1. Therefore,
$$DD_{(a,b)}(G) = np(2n)^a + p(p-n-1)(2n)^a(2)^b.$$ ■

3. THE SECOND GENERALIZED SCHULTZ (OR GUTMAN) INDEX

For any positive real values a and b, the generalized second Schultz index is given by
$$ZZ_{(a,b)}(G) = \sum_{\{u_i,u_j\}\in V(G)} (d(u_i)d(u_j))^a (d(u_i,u_j))^b.$$

Theorem 3.1. *For any connected graph* G *with* $p \geq 3$,
$$\frac{p(p-1)}{2}[\delta(G)]^{2a}[rad(G)]^b \leq ZZ_{(a,b)}(G) \leq \frac{p(p-1)}{2}[\Delta(G)]^{2a}[rad(G)]^b.$$

Proof. Let G be a connected graph with $p \geq 3$. We know that

$$\delta(G)^2 \leq d(u_i).d(u_j) \leq \Delta(G)^2. \tag{19}$$
$$(\delta(G))^{2a} \leq (d(u_i).d(u_j))^a \leq (\Delta(G))^{2a}. \tag{20}$$
$$rad(G) \leq d(u_i, u_j) \leq 2rad(G). \tag{21}$$
$$(rad(G))^b \leq (d(u_i, u_j))^b \leq (2rad(G))^b. \tag{22}$$

Multiplying equations (20) and (22), we have

$$[\delta(G)]^{2a}[rad(G)]^b \leq (d(u_i).d(u_j))^a (d(u_i, u_j))^b \leq [\Delta(G)]^{2a}[2rad(G)]^b.$$
$$\frac{p(p-1)}{2}[\delta(G)]^{2a}[rad(G)]^b \leq ZZ_{(a,b)}(G) \leq \frac{p}{2}(\text{p}-1)^{2a+1}[\Delta(G)]^{2a}2[rad(G)]^b.$$

■

Theorem 3.2. *For any connected graph G with $p \geq 3$,*

$$\frac{p(p-1)}{2}[rad(G)]^b \leq ZZ_{(a,b)}(G) \leq \frac{p}{2}(\text{p}-1)^{2a+1}[2rad(G)]^b.$$

Proof. Let G be a connected graph with $p \geq 3$. We know that

$$1 \leq d(u_i) \leq p-1. \tag{23}$$
$$1 \leq (d(u_i).d(u_j))^a \leq (\text{p}-1)^{2a}. \tag{24}$$
$$(rad(G))^b \leq (d(u_i, u_j))^b \leq (2rad(G))^b. \tag{25}$$

Multiplying equations (24) and (25), we have

$$[rad(G)]^b \leq (d(u_i)d(u_j))^a (d(u_i, u_j))^b \leq (\text{p}-1)^{2a}[2rad(G)]^b.$$
$$\frac{p(p-1)}{2}[rad(G)]^b \leq ZZ_{(a,b)}(G) \leq \frac{p}{2}(\text{p}-1)^{2a+1}[2rad(G)]^b.$$

■

Theorem 3.3. *Let G be any connected graph with $p \geq 3$. Then,*

$$\frac{p(p-1)}{2} \leq ZZ_{(a,b)}(G) \leq \frac{p}{2}(p-1)^{a+b+1}.$$

Proof. Let G be a connected graph with $p \geq 3$. We know that

$$1 \leq (d(u_i).d(u_j))^a \leq (\text{p}-1)^{2a}, \tag{26}$$
$$1 \leq d(u_i, u_j) \leq p-1, \tag{27}$$
$$1 \leq (d(u_i, u_j))^b \leq (p-1)^b. \tag{28}$$

Multiplying equations (26) and (28), we have

$$1 \leq (d(u_i).d(u_j))^a (d(u_i, u_j))^b \leq (\text{p}-1)^a (p-1)^b,$$
$$\frac{p(p-1)}{2} \leq ZZ_{(a,b)}(G) \leq \frac{p}{2}(p-1)^{a+b+1}.$$

■

Theorem 3.4. *For any connected graph G with $p \geq 3$,*

$$\frac{p(p-1)}{2}(\delta(G))^a \leq ZZ_{(a,b)}(G) \leq \frac{p}{2}(\Delta(G))^{2a}(p-1)^{b+1}.$$

Proof. Let G be a connected graph with $p \geq 3$. We know that

$$(\delta(G))^{2a} \leq (d(u_i).d(u_j))^a \leq (\Delta(G))^{2a}. \quad (29)$$

$$1 \leq d(u_i, u_j) \leq p-1. \quad (30)$$

$$1 \leq (d(u_i, u_j))^b \leq (p-1)^b. \quad (31)$$

Multiplying equations (29) and (31), we have

$$\frac{p(p-1)}{2}(\delta(G))^{2a} \leq ZZ_{(a,b)}(G) \leq \frac{p}{2}(\Delta(G))^{2a}(p-1)^{b+1}.$$ ∎

Proposition 3.1. *Let G be the class of some standard graphs. Then,*

(i) $$ZZ_{(a,b)}(C_p) = \begin{cases} 2p(4)^a\left(\frac{(p^2-1)}{8}\right)^b & if\ p\ is\ odd \\ 2p(4)^a\left(\frac{(p-1)^2-1}{8}\right)^b + p(4)^a\left(\frac{p}{2}\right)^b & if\ p\ is\ even \end{cases}.$$

(ii) $ZZ_{(a,b)}(K_p) = p(p-1)^{2a+1}$.

(iii) $ZZ_{(a,b)}(K_{1,p-1}) = (p-1)((p-2)2^b + 2(p-1)^a)$.

(iv) $ZZ_{(a,b)}(W_p) = 2(p-1)((3p-3)^a + 9^a + (p-4)9^a 2^{b-1}$.

Proof. Analogous version from Proposition 2.1 and definition of $ZZ_{(a,b)}(G)$ we have the following results. ∎

Theorem 3.5. *Let $G \cong C_{p1} \circ K_{p2}$ with $p_1 \geq 3$ and $p_2 \geq 1$. Then,*

$$ZZ_{(a,b)}(G) = \begin{cases} p_1p_2(2p_2)^{2a}\left(\frac{p_1}{2}+2\right)^b + p_1(p_2+2)^a\left(\frac{p_1}{2}+1\right)^b & if\ p_2\ is\ odd \\ p_1p_2(2p_2)^{2a}\left(\frac{p_1+2}{2}\right)^b + p_1(p_2+2)^a\left(\frac{p_1+1}{2}\right)^b & if\ p_2\ is\ even \end{cases}.$$

Proof. Let $G \cong C_{p1} \circ K_{p2}$ with $p_1 \geq 3$ and $p_2 \geq 1$. Then, $d(u_i) = p_2 + 2$ for each vertex u_i of cycle C_{p1} and $d(u_j) = p_2$ for each vertex u_j of complete graph K_{p2}.

Case 1. For p_2 is odd, $d(u_i) = \frac{p_1}{2} + 1$ for each vertex u_i of cycle C_{p1} and $d(u_j) = \frac{p_1}{2} + 2$ for each vertex u_j of complete graph K_{p2}. Then,

$$\begin{aligned} ZZ_{(a,b)}(G) &= \sum_{u_i,u_j \in V(G)} (d(u_i).d(u_j))^a (d(u_i,u_j))^b \\ &= p_1p_2(2p_2)^{2a}\left(\frac{p_1}{2}+2\right)^b + p_1(p_2+2)^{2a}\left(\frac{p_1}{2}+1\right)^b \\ &= p_1p_2(2p_2)^{2a}\left(\frac{p_1}{2}+2\right)^b + p_1(p_2+2)^{2a}\left(\frac{p_1+2}{2}\right)^b. \end{aligned}$$

Case 2. For p_2 is odd, $d(u_i) = \frac{p_1-1}{2} + 1$ for each vertex u_i of cycle C_{p1} and $d(u_j) = \frac{p_1-1}{2} + 2$ for each vertex u_j of complete graph K_{p2}. Then,

$$ZZ_{(a,b)}(G) = \sum_{u_i,u_j\in V(G)} (d(u_i).d(u_j))^a (d(u_i,u_j))^b$$
$$= p_1p_2(2p_2)^{2a}\left(\frac{p_1-2}{2}+2\right)^b + p_1(p_2+2)^{2a}\left(\frac{p_1-1}{2}+1\right)^b$$
$$= p_1p_2(2p_2)^{2a}\left(\frac{p_1+2}{2}\right)^b + p_1(p_2+2)^{2a}\left(\frac{p_1+1}{2}\right)^b.$$

■

Theorem 3.6. *Let* $G \cong H_{n,p}$ *be a Harary graph with* $n \geq 2m$*;* $m \geq 1$ *and* $p \geq 4$ *and is even. Then,*

(i) $ZZ_{(a,b)}(G) = 2p(4)^a\left(\frac{(p-1)^2-1}{8}\right)^b + p(4)^a\left(\frac{p}{8}\right)^b$, if $m = 1$.

(ii) $ZZ_{(a,b)}(G) = p(n)^{2a+1} + p(p-n-1)(n)^{2a}(2)^b$, if $n = 2m$; $m \geq 2$.

Proof. By Theorem 2.8, the results (i) and (ii) follow. ■

Theorem 3.7. *Let* $G \cong H_{n,p}$ *be a Harary graph with* $n \geq 2m+1$*;* $m \geq 1$ *and* $p \geq 5$ *and is odd. Then,*

$$ZZ_{(a,b)}(G) = p(n)^{2a+1} + p(p-n-1)(n)^{2a}(2)^b.$$

Proof. By Theorem 2.8, the claim follows. ■

Theorem 3.8. (***Radon's inequality***) [13] *For real numbers* $t > 0$, $x_1, x_2, \ldots, x_s > 0$, $a_1, a_2, \ldots, a_s > 0$*, then following inequality holds*:

$$\sum_{n=1}^{s} \frac{x_n^{t+1}}{a_n^t} \geq \frac{(\sum_{n=1}^{s} x_n)^{t+1}}{(\sum_{n=1}^{s} a_n)^t}.$$

Now, we use the Radon's inequality to give the relation between $DD_{(a,b)}(G)$ and $ZZ_{(a,b)}(G)$.

Theorem 3.9. *Let* G *be a connected graph with* $p \geq 3$ *and is odd. Then,*

$$\Delta(G)\delta(G)DD_{(a,b)}(G) \leq \left(\Delta(G)+\delta(G)\right)^2 ZZ_{(a,b)}(G)(W(G))^b.$$

Proof. Let each n in Theorem 3.9 corresponds to the vertex pair (u_i, u_j) with $s = \frac{p(p-1)}{2}$ and $t = 1$. Then each x_n is replaced by $(d(u_i) + d(u_j))^a (d(u_i,u_j))^b$ and a_n is replaced by $(d(u_i).d(u_j))^a (d(u_i,u_j))^b$. Thus,

$$\frac{\left(\sum_{i<j}(d(u_i)+d(u_j))^a(d(u_i,u_j))^b\right)^2}{\sum_{i<j}(d(u_i).d(u_j))^a(d(u_i,u_j))^b} \le \sum_{i<j}\frac{(d(u_i)+d(u_j))^a}{(d(u_i).d(u_j))^a}(d(u_i,u_j))^b,$$

$$\frac{DD_{(a,b)}(G)^2}{ZZ_{(a,b)}(G)} \le \sum_{i<j}\left(\sqrt{\frac{d(u_i)}{d(u_j)}}+\sqrt{\frac{d(u_j)}{d(u_i)}}\right)^2 (d(u_i,u_j))^b,$$

$$\left(\sqrt{\frac{d(u_i)}{d(u_j)}}+\sqrt{\frac{d(u_j)}{d(u_i)}}\right)^2 \le \frac{(\Delta(G)+\delta(G))^2}{(\Delta(G)\delta(G))}.$$

Therefore,

$$\frac{DD_{(a,b)}(G)^2}{ZZ_{(a,b)}(G)} \le \frac{(\Delta(G)+\delta(G))^2}{(\Delta(G)\delta(G))}\left(d(u_i,u_j)\right)^b. \qquad \blacksquare$$

4. THE FIRST GENERALIZED SCHULTZ POLYNOMIALS

For any positive real number a and b, the first generalized Schultz polynomial of a graph G is given by

$$DD_{(a,b)}(G,x) = \sum_{i<j}(d(u_i)+d(u_j))^a\, x^{(d(u_i,u_j))^b},$$

where $(d(u_i,u_j))^b$ denotes the distance between the pair of the vertices and $d(u_i)$ denotes the degree of the vertex u_i.

Observation 4.1.

(i) The $DD_{(a,b)}(G,x)$ has no constant terms.

(ii) Derivatives of the $DD_{(a,b)}(G,x)$ is the degree distance index of the graph at $x=1$.

Observation 4.2. Let G be the class of standard graphs. Then

(i) $DD_{(a,b)}(C_p,x) = \frac{(4p)^a(1-x^{\left(\frac{p+2}{2}\right)^b})}{1-x}$.

(ii) $DD_{(a,b)}(K_p,x) = (2p(p-1))^a x$.

(iii) $DD_{(a,b)}(K_{1,p-1},x) = \left(p(p-1)\right)^a x + \left\lfloor\frac{p}{2}\right\rfloor(p-1)x^{2^b}$.

(iv) $DD_{(a,b)}(W_{1,p-1},x) = 2(p-1)((p-2)^a+6^a)x$
$+ 2(p-1)((p-4)6^a)x^{2^{b-1}}$.

Theorem 4. 1. *Let* $G \cong C_{p1}\circ K_{p2}$ *with* $p_1 \ge 3$ *and* $p_2 \ge 2$. *Then,*

$$DD_{(a,b)}(G,x) = \begin{cases} p_1p_2(2p_2)^2\left(\frac{1-x^{\left(\frac{p_1}{2}+3\right)^b}}{1-x}\right) + p_1(2p_2+4)^a\left(\frac{1-x^{\left(\frac{p_1}{2}+2\right)^b}}{1-x}\right) \; if\ p_2\ is\ even \\ p_1p_2(2p_2)^a\left(\frac{1-x^{\left(\frac{p_1+4}{2}\right)^b}}{1-x}\right) + p_1(2p_2+4)^a\left(\frac{1-x^{\left(\frac{p_1+3}{2}\right)^b}}{1-x}\right) \; if\ p_2\ is\ odd \end{cases}.$$

Proof. Let $G \cong C_{p1} \circ K_{p2}$ with $p_1 \geq 3$ and $p_2 \geq 2$.Then, $d(u_i) = p_2 + 2$ for each vertex u_i of cycle C_{p1} and $d(u_i) = p_2 + 2$ for each vertex u_j of complete graph K_{p2} is $d(u_j) = p_2$.

Case 1. For p_2 is even, for each vertex u_i of cycle the distance is $\frac{p_1}{2} + 1$ and for each vertex u_j of complete graph K_{p2} the distance is $\frac{p_1}{2} + 2$. Therefore,

$$\begin{aligned} DD_{(a,b)}(G,x) &= \sum_{u_i,u_j \in V(G)} (d(u_i) + d(u_j))^a x^{(d(u_i,u_j))^b} \\ &= \sum_{i=1}^{\frac{p_1+2}{2}} p_1p_2(2p_2)^a x^i + \sum_{i=1}^{\frac{p_1+1}{2}} p_1(2(p_2+2))^a x^i \\ &= p_1p_2(2p_2)^2\left(\frac{1-x^{\left(\frac{p_1}{2}+3\right)^b}}{1-x}\right) + p_1(2p_2+4)^a\left(\frac{1-x^{\left(\frac{p_1}{2}+2\right)^b}}{1-x}\right). \end{aligned}$$

Case 2. Suppose that p_2 is odd, then for each vertex u_i of cycle C_{p1} the distance is $\frac{p_1-1}{2} + 1$ and for each vertex u_j of complete graph K_{p2} the distance is $\frac{p_1-1}{2} + 2$. Then,

$$\begin{aligned} DD_{(a,b)}(G,x) &= \sum_{u_i,u_j \in V(G)} (d(u_i).d(u_j))^a x^{(d(u_i,u_j))^b} \\ &= \sum_{i=1}^{\frac{p_1-1}{2}+2} p_1p_2(2p_2)^a x^i + \sum_{i=1}^{\frac{p_1-1}{2}+2} p_1(2(p_2+2))^a x^i \\ &= p_1p_2(2p_2)^a\left(\frac{1-x^{\left(\frac{p_1+4}{2}\right)^b}}{1-x}\right) + p_1(2p_2+4)^a\left(\frac{1-x^{\left(\frac{p_1+3}{2}\right)^b}}{1-x}\right). \end{aligned}$$

■

Theorem 4.2. *Let $G \cong H_{n,p}$ be a Harary graph with $n \geq 2m, m \geq 1$ and $p \geq 4$ and is even. Then,*

(i) $DD_{(a,b)}(H_{n,p},x) = 2p(4)^a\left(\frac{1-x^{\left(\frac{p+2}{2}\right)^b}}{1-x}\right)$, if $m = 1$.

(ii) $DD_{(a,b)}(H_{n,p},x) = np(2n)^a x + p(p-n-1)(2n)^a x^{2^b}$, if $n = 2m, m \geq 2$.

Proof. (i) If $H_{n,p}$ is a 2-regular graph. The maximum distance of the graph is $\left\lfloor \frac{p}{2} \right\rfloor$. The degree sequence will be $(2, 2, \ldots, 2)$. Therefore,

$$DD_{(a,b)}(G,x) = \sum_{u_i,u_j \in V(G)} (d(u_i) + d(u_j))^a x^{(d(u_i,u_j))^b}$$

$$= \sum_{i=1}^{\frac{p}{2}} 2p(4)^a x^i = 2p(4)^a \left(\frac{1-x^{\left(\frac{p+2}{2}\right)^b}}{1-x} \right).$$

(ii) If $H_{n,p}$ is $r-$regular and p times of $(p-n-1)$ vertices are at the maximum distance at 2 and all other vertices at the distance 1. Then,

$$DD_{(a,b)}(G,x) = \sum_{u_i,u_j \in V(G)} (d(u_i)d(u_j))^a x^{(d(u_i,u_j))^b}$$

$$DD_{(a,b)}(H_{n,p},x) = np(2n)^a x + p(p-n-1)(2n)^a x^{2^b}.$$

■

5. THE SECOND GENERALIZED SCHULTZ POLYNOMIALS

For any positive real numbers a and b, the second Generalized Schultz (Gutman) polynomial of a graph G is given by

$$ZZ_{(a,b)}(G,x) = \sum_{i<j} (d(u_i)d(u_j))^a \, x^{(d(u_i,u_j))^b}.$$

where $(d(u_i,u_j))^b$ denotes the distance between the pair of the vertices and $d(u_i)$ denotes the degree of the vertex u_i.

Observation 5.1.

(i) The $ZZ_{(a,b)}(G,x)$ has no constant terms.

(ii) Derivatives of the $ZZ_{(a,b)}(G,x)$ is the degree distance index of the graph at $x = 1$.

Observation 5.2. Let G be the class of standard graphs. Then

(i) $ZZ_{(a,b)}(C_p,x) = \frac{(4p)^a\left(1-x^{\left(\frac{p+2}{2}\right)^b}\right)}{1-x}$.

(ii) $ZZ_{(a,b)}(K_p,x) = p(p-1)^{2a}x$.

(iii) $ZZ_{(a,b)}(K_{1,p-1},x) = (p-1)^{2a}x + \binom{p-1}{2}x^{2^b}$.

(iv) $ZZ_{(a,b)}(W_{1,p-1},x) = 2(p-1)((3p-3)^a + 9^a)x + 2(p-1)((p-4)6^a)x^{2^{b-1}}$.

Theorem 5. 1. *Let* $G \cong C_{p1} \circ K_{p2}$ *with* $p_1 \geq 3$ *and* $p_2 \geq 2$. *Then,*

$$ZZ_{(a,b)}(G,x) = \begin{cases} p_1p_2(2p_2)^{2a}\left(\frac{1-x^{\left(\frac{p_1}{2}+3\right)^b}}{1-x}\right) + p_1(p_2+2)^a\left(\frac{1-x^{\left(\frac{p_1}{2}+2\right)^b}}{1-x}\right) if\ p_2\ is\ even \\ p_1p_2(2p_2)^{2a}\left(\frac{1-x^{\left(\frac{p_1+4}{2}\right)^b}}{1-x}\right) + p_1(p_2+2)^a\left(\frac{1-x^{\left(\frac{p_1+3}{2}\right)^b}}{1-x}\right) if\ p_2\ is\ odd \end{cases}.$$

Proof. By Theorem 4.1, the desired result follows. ■

Theorem 5.2. *Let* $G \cong H_{n,p}$ *be a Harary graph with* $n \geq 2m$. $m \geq 1$ *and* $p \geq 4$ *and is even. Then,*

(i) $ZZ_{(a,b)}(H_{n,p},x) = 2p(4)^a\left(\frac{1-x^{\left(\frac{p+2}{2}\right)^b}}{1-x}\right)$, if $m = 1$.

(ii) $ZZ_{(a,b)}(H_{n,p},x) = p(n)^{2a+1}x + p(p-n-1)(n)^{2a}x^{2^b}, if\ n = 2m;\ m \geq 2.$

Proof. By Theorem 4.2, the desired result follows. ■

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