Some Properties of Generalized Schultz and Generalized Modified Schultz Distances

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We greatly appreciate the valuable input and feedback on our revised work. We have further refined our article in response to these new comments. We have seen that these comments have significantly enhanced the caliber of our work. We trust that this amended document adequately resolves all the concerns raised, and eagerly anticipate a positive judgment in the near future.

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Abstract The Schultz topological index is a degree-distance-based topological descriptor that can be obtained from a certain connected graph. It was proposed by Schultz in 1989. This index can predict the physical properties of chemical compounds, such as boiling point and others. Chemical and physical properties of chemical compounds, such as boiling point and others, can be predicted by this index. And it was later modified by Klavžar and Gutman in 1997, Gutman defined the Schultz and modified Schultz polynomials in 2005. With respect to this generalization. This article presents a generalization to Schultz and modified Schultz distances and defines the corresponding indices, polynomials, and averages. Furthermore, the polynomials of the Schultz and modified Schultz distances generalized to a wheel graph were obtained, along with some properties related to this type of distance.

1 Introduction

Given a finite simple indirectly connected graph Φ , $V(\Phi)$ represents the vertices set of Φ and $E(\Phi)$ represents the edges set of Φ , the distance between any two vertices $u, v \in V(\Phi)$, $u \neq v$ is the length of the shortest path between them and denoted by d(u,v), $\delta(v)$ (or degv) is the degree of the vertex v [1]. In graph theory, there are numerous topological indices, the first one is the Wiener index, which was presented by Harry Wiener in 1947 [2], and defined it as follows:

$$W(\Phi) = \sum_{\{v,u\} \subseteq V(\Phi)} d(v,u)$$

Then the scientist Haruo Hosoya in 1988 defined the Wiener polynomial, which was later called the Hosoya polynomial [3], as follows:

$$H\left(G;x\right) = \sum_{\{v,u\}\subseteq V(G)} x^{d(v,u)}$$

There is another topological index called The Schultz index, The Shultz index is a numerical parameter of a connected graph, and serves as a topological invariant, it is utilized to study the physical and chemical properties of chemical compounds [4]. The Shultz index was introduced by Schultz in 1989 [5], and it is defined as:

$$Sc(\Phi) = \sum_{\{v,u\}\subseteq V(\Phi)} \left(degv + degu\right) d\left(v,u\right).$$

Klavžar and Gutman defined the modified Schultz index in 1997 [6], as follows:

In 2005 [7] Gutman defined Schultz and modified Schultz polynomials respectively as:

$$\begin{aligned} Sc\left(\Phi;x\right) &= \sum_{\{u,v\}\subseteq V(\Phi)} \left(degv + degu\right) x^{d(u,v)}.\\ Sc^*\left(\Phi;x\right) &= \sum_{\{u,v\}\subseteq V(\Phi)} \left(degv \times degu\right) x^{d(u,v)}. \end{aligned}$$

The average Schultz and modified Schultz distances are introduced by Ahmed and Haitham [8], respectively as:

$$\overline{Sc}(\Phi) = 2Sc(\Phi) / p(p-1).$$
$$\overline{Sc^*}(\Phi) = 2Sc^*(\Phi) / p(p-1).$$

Several papers have contributed to calculating Schultz and modified Schultz polynomials for different graphs, for more information see references [9, 10, 11]. Additionally, there is a lot of applications of Schultz and modified Schultz indices in Chemistry [12, 13, 14]. There are also other topological indices and other polynomials that have been found by several researchers [15, 16, 17]. In the following section, generalizations for Schultz and modified Schultz distances are given, also, and the polynomial, the index and the average distance were given for each type of this generalization.

2 Generalizing Schultz and modified Schultz distances

Definition 1. Let Φ be a simple connected graph and let $d^{GS}(u, v)$ be the generalized Schultz distance between any distinct vertices v and u of Φ which is defined by:

$$d^{GS}\left(v,u\right) = min_{Q}\left[\left\{ degv + \alpha \sum_{w \in V(Q) - \{v,u\}} degw + degu \right\} l(Q)\right],$$

where Q is any path between u and v, the minimum is taken over all (v, u) – paths Q, degy is a degree of any vertex y in V(Q) and $\alpha \in \{0, 1\}$. If $\alpha = 0$, then generalized Schultz distance is equal to Schultz distance.

We can rewrite the generalized Schultz distance $d^{GS}(v, u)$ as:

$$d^{GS}(v,u) = min_Q\left[\left\{\sum_{w \in V(Q)} degw\right\} l(Q)\right],\tag{2.1}$$

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where Q is any (v, u) – path, the minimum is taken over all (v, u) – paths Q and degw is a degree of vertex w.

The generalized Shultz polynomial is defined as:

 $GSc(\Phi; x) = \sum_{\{v,u\} \subseteq V(\Phi)} S_d(v, u, Q) x^{l(Q)}$, where $S_d(v, u, Q) = \frac{d^{GS}(v, u)}{l(Q)}$. We can also write this polynomial in another form:

$$GSc(\Phi; x) = \sum_{k \ge 1} S_d(\Phi, k) x^k, \qquad (2.2)$$

where $S_d(\Phi, k)$ is the sum degrees of all vertices in a (v, u) – path $Q, v, u \in V(\Phi)$ that satisfy the condition (1) at $l(Q) = k, k \ge 1$.

Now, the generalized Schultz index is defined as:

$$GSc(\Phi) = \frac{d}{dx} \left(GSc(\Phi; x) \right) |_{x=1}$$
$$= \sum_{k \ge 1} kS_d(\Phi, k) = \sum_{\{u,v\} \subseteq V(\Phi)} d^{GS}(v, u).$$
(2.3)

The generalizations of the Schultz polynomial and Schultz index of a vertex v are defined respectively as:

$$GSc(v, \Phi; x) = \sum_{u \in V(\Phi) - \{v\}} S_d(v, u, Q) x^{l(Q)} = \sum_{k \ge 1} S_d(v, G, k) x^k,$$

where $S_d(v, \Phi, k)$ is the sum degrees of all vertices in a (v, u) – path $Q, u \in V(\Phi) - \{v\}$ that satisfy the condition (2.1) at $l(Q) = k, k \ge 1$. The index of a vertex v with respect to this generalization is

$$GSc(v, \Phi) = \frac{d}{dx} \left(GSc(v, \Phi; x) \right) |_{x=1}$$
$$= \sum_{k \ge 1} kS_d(v, G, k) = \sum_{u \in V(\Phi) - \{v\}} d^{GS}(v, u).$$

Hence,

$$\begin{split} GSc\left(\Phi;x\right) &= \frac{1}{2}\sum_{v\in V(G)}GSc\left(v,\Phi;x\right).\\ GSc\left(\Phi\right) &= \frac{1}{2}\sum_{v\in V(\Phi)}GSc\left(v,\Phi\right). \end{split}$$

The average of this type of distance is defined as:

 $\overline{GSc}(\Phi) = 2GSc(\Phi)/p(p-1)$, where p is an order of a connected graph Φ .

Definition 2. Let Φ be a connected graph and let $d^{GS^*}(v, u)$ be the generalized modified Schultz distance between any distinct vertices v and u of Φ which is defined by:

$$d^{GS^*}(v,u) = \min_{Q} \left[\left\{ degv \times \alpha \prod_{w \in V(Q) - \{u,v\}} degw \times degu \right\} l(Q) \right],$$

where Q is any (v, u) – path, the minimum is taken over all (v, u) – paths Q, degy is a degree of any vertex y in V(Q) and $\alpha \in \{0,1\}$. If $\alpha = 0$, then the generalized modified Schultz distance is equal modified Schultz distance.

We can rewrite the modified generalized Schultz distance $d^{GS^*}(v, u)$ as:

$$d^{GS^*}(v,u) = min_Q\left[\left\{\prod_{w \in V(Q)} degw\right\} l(Q)\right],\tag{2.4}$$

where Q is any (v, u) – path, the minimum is taken over all (v, u) – paths Q and degw is a degree of vertex w.

The generalized modified Shultz polynomial is defined as:

 $GSc^*(\Phi; x) = \sum_{\{v,u\} \subseteq V(G)} S_d^*(v, u, Q) x^{l(Q)}, \text{ where } S_d^*(v, u, Q) = \frac{d^{GS^*}(v, u)}{l(Q)}.$ We can also write this polynomial in another form as:

$$GSc^{*}(\Phi; x) = \sum_{k \ge 1} S_{d}^{*}(\Phi, k) x^{k},$$
(2.5)

where $S^*_d(G,k)$ is the sum degrees of all vertices in a (v,u) – path Q and $v,u \in V(\Phi)$ that satisfy the condition (2.4) at $l(Q) = k, k \ge 1$.

Now, the generalized modified Schultz index is defined as:

$$GSc^{*}(\Phi) = \frac{d}{dx} (GSc^{*}(\Phi; x))|_{x=1}$$
$$= \sum_{k \ge 1} kS_{d}^{*}(\Phi, k) = \sum_{\{v, u\} \subseteq V(\Phi)} d^{GS^{*}}(v, u).$$
(2.6)

The generalizations of the modified Shultz polynomial and modified Schultz index of a vertex v are defined respectively as:

$$GSc^*(v, \Phi; x) = \sum_{u \in V(\Phi) - \{v\}} S_d^*(v, u, Q) x^{l(Q)} = \sum_{k \ge 1} S_d^*(v, \Phi, k) x^k,$$

where $S_d^*(v, \Phi, k)$ is the sum degrees of all vertices in a (v, u) – path Q, $u \in V(\Phi) - \{v\}$ that satisfy the condition (2.4) at l(Q) = k, $k \ge 1$. The index of a vertex v with respect to this generalization is:

$$GSc^{*}(v, \Phi) = \frac{d}{dx} (GSc^{*}(v, \Phi; x))|_{x=1}$$
$$= \sum_{k \ge 1} k S_{d}^{*}(v, \Phi, k) = \sum_{u \in V(\Phi) - \{v\}} d^{GS^{*}}(v, u).$$

Hence,

$$GSc^*(\Phi; x) = \frac{1}{2} \sum_{v \in V(\Phi)} GSc^*(v, \Phi; x).$$
$$GSc^*(\Phi) = \frac{1}{2} \sum_{v \in V(\Phi)} GSc^*(v, \Phi).$$

The average of generalized modified Schultz distance is defined as:

 $\overline{GSc^*}(\Phi) = 2GSc^*(\Phi)/p(p-1)$, where p is an order of a connected graph Φ .

3 Some Properties of Generalized Schultz and Modified Schultz distances

Let $S(\Phi, k)$ and $S^*(\Phi, k)$ be the sum of degv + degu and $degv \times degu$ of all (v, u) – paths of length k respectively, then

3.1 The generalized of Schultz and modified Schultz distances between any two adjacent vertices in the graph Φ is equal to Schultz and modified Schultz distances, respectively, therefore:

$$S_d(\Phi, 1) = S(\Phi, 1),$$

 $S_d^*(\Phi, 1) = S^*(\Phi, 1).$

If Φ is a connected graph of diameter one, then:

- (i) $GSc(\Phi; x) = Sc(\Phi; x)$.
- (ii) $GSc^*(\Phi; x) = Sc^*(\Phi; x)$.

Example 3.1 Let K_p be a complete graph of order $p, p \ge 2$, then:

$$GSc(K_p; x) = Sc(K_p; x) = p(p-1)^2 x,$$

$$GSc^*(K_p; x) = Sc^*(K_p; x) = \frac{1}{2}p(p-1)^3 x$$

- **3.2** If Φ is a tree graph, then the minimum in generalized Schultz and modified Schultz distances are not important because there is only one path between any two vertices in the tree graph, so it can be removed.
- **3.3** In a connected graph Φ , if there is a common vertex of degree h from which all paths of length 2 pass, to which the generalized Schultz and modified Schultz distances apply, let its number be n, then:

$$S_d(\Phi, 2) = S(\Phi, 2) + nh,$$

$$S_d^*(\Phi, 2) = S^*(\Phi, 2) \times h.$$

Example 3.2. Let S_p be a star graph of order p, where $p \ge 4$, then:

(i)
$$GSc(S_p; x) = Sc(S_p; x) + n \times hx^2$$

$$= p(p-1)x + (p-1)(p-2)x^2 + \frac{(p-1)(p-2)}{2} \times (p-1)x^2$$

$$= p(p-1)x + \frac{1}{2}(p^2 - 1)(p-2)x^2.$$
(ii) $GSc^*(S_p; x) = Sc^*(S_p; x) \times h - S^*(S_p, 1) \times (h-1)x$

$$= \left[(p-1)^2x + \frac{1}{2}(p-1)(p-2)x^2\right] \times (p-1) - (p-1)^2(p-2)x$$

$$= (p-1)^2x + \frac{1}{2}(p-1)^2(p-2)x^2.$$

Example 3.3. Let F_p be a fan graph of order p, where p = 2i + 1, for all $i \in N - \{1\}$, then

(i) $GSc(F_p; x) = Sc(F_p; x) + n \times hx^2$

. . .

$$= (p-1) (p+3) x + 2 (p-1) (p-3) x^{2} + \frac{1}{2} (p-3) (p-1) (p-1) x^{2}$$
$$= (p-1) (p+3) x + \frac{1}{2} (p-1) (p^{2}-9) x^{2}.$$

So $c^{*}(F_{p}; x) = Sc^{*}(F_{p}; x) \times h - S^{*}(F_{p}, 1) \times (h-1) x$

(ii)
$$GSc^*(F_p; x) = Sc^*(F_p; x) \times h - S^*(F_p, 1) \times (h - 1) x$$

= $[2p(p-1)x + 2(p-3)(p-1)x^2](p-1) - 2p(p-1)(p-2)x$
= $2p(p-1)x + 2(p-3)(p-1)^2x^2$.

3.4 If Φ is the *r*-regular graph, then:

- (i) $GSc(\Phi; x) = \sum_{\{u,v\} \subseteq V(\Phi)} r(l(Q) + 1) x^{l(Q)}$.
- (ii) $GSc^*(\Phi; x) = \sum_{\{u,v\} \subseteq V(\Phi)} r^{(l(Q)+1)} x^{l(Q)}.$

Where Q is the shortest path between any two vertices u and v in the graph Φ of length l(Q). **Proof:**

(i) From definition of generalized Schultz polynomial, we get

$$\begin{split} GSc\left(\Phi;x\right) &= \sum_{\{u,v\}\subseteq V(\Phi)} \left(degu + \sum_{w\in V(Q)-\{u,v\}} degw + degv\right) x^{l(Q)} \\ &= \sum_{\{u,v\}\subseteq V(\Phi)} \left(r + \sum_{w\in V(Q)-\{u,v\}} r + r\right) x^{l(Q)} \\ &= \sum_{\{u,v\}\subseteq V(\Phi)} \left(r + r(l(Q) - 1) + r\right) x^{l(Q)} \\ &= \sum_{\{u,v\}\subseteq V(\Phi)} r(l(Q) + 1) x^{l(Q)}. \end{split}$$

Where Q is the shortest path between any two vertices u and v in the graph Φ of length l(Q).

(ii) $GSc^*(\mathbf{G}; x) = \sum_{\{u,v\} \subseteq V(\Phi)} (degu \times \prod_{w \in V(Q) - \{u,v\}} degw \times degv) x^{l(Q)}$

$$= \sum_{\{u,v\}\subseteq V(\Phi)} (r \times \prod_{w\in V(Q)-\{u,v\}} r \times r) x^{l(Q)}$$
$$= \sum_{\{u,v\}\subseteq V(\Phi)} (r \times r^{l(Q)-1} \times r) x^{l(Q)}$$
$$= \sum_{\{u,v\}\subseteq V(\Phi)} r^{l(Q)+1} x^{l(Q)}.$$

Where Q is the shortest path between any two vertices u and v in the graph Φ of length l(Q).

3.5 If the connected graph Φ is the *r*-regular, then:

=

- (i) $GSc(\Phi; x) = \frac{d}{dx}(rxH(\Phi; x)).$
- (ii) $GSc^*(\Phi; x) = rH(\Phi; rx).$

Proof:

Since Φ is the *r*-regular connected graph, then: l(Q) = d(v, u), for all (v, u) – path Q is satisfied generalized of Schultz and modified Schultz distances in Φ , $v, u \in V(\Phi)$, then:

(i) $d^{GS}(u,v) = (l(Q) + 1) r l(Q)$. Therefore,

$$GSc(\Phi; x) = \sum_{l(Q) \ge 1} S_d(\Phi, l(Q)) x^{l(Q)}$$

$$=\sum_{l(Q)\geq 1} \left(l(Q)+1\right) r d\left(\Phi,l(Q)\right) x^{l(Q)},$$

where $d(\Phi, l(Q))$ is the number of paths of length l(Q), for all $l(Q) \ge 1$, then:

$$GSc(\Phi; x) = r \sum_{l(Q) \ge 1} l(Q)d(\Phi, l(Q)) x^{l(Q)} + r \sum_{l(Q) \ge 1} d(\Phi, l(Q)) x^{l(Q)}$$

= $rx \frac{d}{dx} (\sum_{l(Q) \ge 1} d(\Phi, l(Q)) x^{l(Q)}) + r \sum_{l(Q) \ge 1} d(\Phi, l(Q)) x^{l(Q)}$
= $rx \frac{d}{dx} H(\Phi; x) + rH(\Phi; x)$
= $\frac{d}{dx} (rxH(\Phi; x)).$

(ii) $d^{GS^*}(u,v) = r^{l(Q)+1} l(Q)$. Therefore,

$$GSc(\Phi; x) = \sum_{(Q) \ge 1} S_d^*(\Phi, l(Q)) x^{(Q)}$$
$$= \sum_{l(Q) \ge 1} r^{l(Q)+1} d(\Phi, l(Q)) x^{l(Q)},$$

where $d(\Phi, l(Q))$ is the number of paths of length l(Q), for all $l(Q) \ge 1$, then

$$GSc^{*}(\Phi; x) = r \sum_{l(Q) \ge 1} d(\Phi, l(Q))(rx)^{l(Q)}$$
$$= rH(G; rx)$$

Remark 3.4. Hosoya polynomial of a cycle graph C_p of order $p, p \ge 3$, [3] is

$$H\left(C_{p};x\right) = \sum_{k=1}^{\left\lfloor \frac{p}{2} \right\rfloor-1} px^{k} + \begin{cases} \frac{p}{2}x^{\frac{p}{2}} & , \ p \ge 4 \ , \ p = 2\left\lceil \frac{p}{2} \right\rceil, \\ 0 & , \ p \ge 3, \ p \ne 2\left\lceil \frac{p}{2} \right\rceil.$$

Example 3.5. Let C_p be a cycle graph of order p, then

- (i) $GSc(C_p; x) = \frac{d}{dx}(2xH(C_p; x)),$
 - a. If p is an odd number, where $p \ge 3$, then

$$GSc(C_p; x) = \frac{d}{dx} (2p \sum_{k=1}^{\left\lceil \frac{p}{2} \right\rceil - 1} x^{k+1}) = 2p \sum_{k=1}^{\left\lceil \frac{p}{2} \right\rceil - 1} (k+1) x^k.$$

b. If p is an even number, where $p \ge 4$, then

$$GSc(C_p; x) = \frac{d}{dx} (2p \sum_{k=1}^{\lceil \frac{p}{2} \rceil - 1} x^{k+1} + px^{\frac{p}{2} + 1})$$
$$= 2p \sum_{k=1}^{\lceil \frac{p}{2} \rceil - 1} (k+1) x^k + p(\frac{p}{2} + 1) x^{\frac{p}{2}}.$$

(ii) $GSc^*(C_p; x) = 2H(C_p; 2x).$ Since $H(C_p; 2x) = p \sum_{k=1}^{\left\lceil \frac{p}{2} \right\rceil - 1} 2^k x^k + \begin{cases} \frac{p}{2} (2x)^{\frac{p}{2}} , & p \ge 4, \ p = 2 \left\lceil \frac{p}{2} \right\rceil, \\ 0, & p \ge 3, \ p \ne 2 \left\lceil \frac{p}{2} \right\rceil. \end{cases}$ Then

Then

$$GSc^{*}(C_{p};x) = 2p \sum_{k=1}^{\left\lceil \frac{p}{2} \right\rceil - 1} 2^{k} x^{k} + \begin{cases} 2^{\frac{p}{2}} p x^{\frac{p}{2}} &, p \ge 4, p = 2 \left\lceil \frac{p}{2} \right\rceil, \\ 0 &, p \ge 3, p \ne 2 \left\lceil \frac{p}{2} \right\rceil. \end{cases}$$

Remark 3.6. For any r-regular connected graph Φ , then

(i) $H(\Phi; x) = Sc(\Phi; x)/2r$, [8]. Since, $GSc(\Phi; x) = \frac{d}{dx}(rxH(\Phi; x))$, then

$$GSc(\Phi; x) = \frac{d}{dx} \left(rxSc(\Phi; x) / 2r \right)$$
$$= \frac{1}{2} \frac{d}{dx} \left(xSc(\Phi; x) \right).$$

(ii)
$$H(\Phi; x) = Sc^*(\Phi; x) / r^2$$
, [8].
Since, $GSc^*(\Phi; x) = rH(\Phi; rx)$, then

$$GSc^* (\Phi; x) = rSc^* (\Phi; rx) / r^2$$
$$= Sc^* (\Phi; rx) / r.$$

Corollary 3.7. For any *r*-regular connected graph Φ , then

(i)
$$GSc(\Phi; x) = \frac{1}{2} \frac{d}{dx} (xSc(\Phi; x)).$$

(ii)
$$GSc^*(\Phi; x) = \frac{1}{r}Sc^*(\Phi; rx)$$
.

Example 3.8. Let G be a Peterson graph (3-regular), of order 10 and size 15, then

(i) $GSc(G; x) = 90x + 270x^2$.

(ii) $GSc^*(G; x) = 135x + 810x^2$.

Solution:

Since Schultz polynomial for Peterson graph G is $Sc(G; x) = 90x + 180x^2$, then

$$GSc(G;x) = \frac{1}{2}\frac{d}{dx}(xSc(G;x))$$
$$= 90x + 270x^{2}.$$

Since the modified Schultz polynomial for Peterson graph G is $Sc^*(G; x) = 135x + 270x^2$, then

$$GSc^*(G; x) = \frac{1}{3}Sc^*(G; 3x)$$

= 135x + 810x².

3.6 Let Φ be any simple connected graph, not a complete graph, then

(i) $Sc(\Phi; 1) < GSc(\Phi; 1)$.

(ii) $Sc^*(\Phi; 1) < GSc^*(\Phi; 1)$.

Proof:

(i) From the definition of generalized Schultz polynomial, we get

$$GSc(\Phi;1) = \sum_{\{u,v\}\subseteq V(\Phi)} (degu + \sum_{w\in V(Q)-\{u,v\}} degw + degv)$$
$$= \sum_{\{u,v\}\subseteq V(\Phi)} (degu + degv) + \sum_{\{u,v\}\subseteq V(\Phi)} \sum_{w\in V(Q)-\{u,v\}} degw$$
$$= Sc(\Phi;1) + \sum_{\{u,v\}\subseteq V(\Phi)} \sum_{w\in V(Q)-\{u,v\}} degw.$$

Since $\sum_{\{u,v\}\subseteq V(\Phi)} \sum_{w\in V(Q)-\{u,v\}} degw \ge 2$, then

$$Sc(\Phi;1) < GSc(\Phi;1)$$
.

(ii) From the definition of generalized modified Schultz polynomial, we get

$$GSc^*\left(\Phi;1
ight) = \sum_{\{u,v\}\subseteq V(\Phi)} (degu imes \prod_{w\in V(Q)-\{u,v\}} degw imes degv).$$

Since $\prod_{w \in V(Q) - \{u,v\}} degw \ge 2$, then

 $Sc^{*}(\Phi; 1) < GSc^{*}(\Phi; 1)$.

Remark 3.9. If Φ is a complete graph, then

(i)
$$Sc(\Phi; 1) = GSc(\Phi; 1)$$
.

(ii) $Sc^{*}(\Phi; 1) = GSc^{*}(\Phi; 1).$

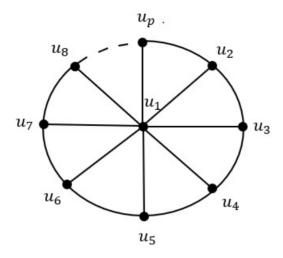


Figure 1. Wheel Graph

Table 1. Generalized Schultz and generalized modified Schultz polynomials and indices of a wheel graph W_p , $4 \le p \le 14$

$p, r \leq p \leq 1 + $				
p	$GSc \ (W_p; x)$	$GSc \ (W_p)$	GSc^* $(W_p; x)$	$GSc^{*}\left(W_{p}\right)$
4	36 <i>x</i>	36	54 <i>x</i>	54
5	$52x + 18x^2$	88	$84x + 54x^2$	192
6	$70x + 45x^2$	160	$120x + 135x^2$	390
7	$90x + 90x^2$	270	$162x + 324x^2$	810
8	$112x + 154x^2$	420	$210x + 630x^2$	1470
9	$136x + 240x^2$	616	$264x + 1080x^2$	2424
10	$162x + 351x^2$	864	$324x + 1701x^2$	3726
11	$190x + 490x^2$	1170	$390x + 2520x^2$	5430
12	$220x + 660x^2$	1540	$462x + 3564x^2$	7590
13	$252x + 864x^2$	1980	$540x + 4860x^2$	10260
14	$286x + 858x^2 + 156x^3$	2470	$624x + 6335x^2$	13494

4 Generalized Schultz and Modified Schultz Polynomials for a Wheel Graph

The Wheel Graph W_p is a graph consisting of a cycle graph of (p-1) vertices, $p \ge 4$ with one central vertex adjacent to all the vertices of the cycle.

It is not easy to find generalized Schultz and generalized modified Shultz polynomials for a wheel graph W_p , $p \ge 4$ in a general form, but we can find a general form of generalized Schultz and generalized modified Schultz polynomials of W_p , $p \ge 15$. The table below shows the generalized Schultz and generalized modified Schultz polynomials and indices for a wheel graph W_p , $4 \le p \le 14$.

Theorem 4.1. Let W_p be a wheel graph of order $p, p \ge 14$, then

$$GSc (W_p; x) = (p-1) (p+8) x + \frac{1}{2} (p-1)((p-2(j+1))(p+5) + 18) x^2 + (p-1) \sum_{k=3}^{j} 3(k+1) x^k, j = \left\lfloor \frac{-3 + \sqrt{129 + 24p}}{6} \right\rfloor.$$

Proof:

Let $V(W_p) = \{u_1, u_2, \ldots, u_p\}$, where $degu_1 = p - 1$ and $degu_i = 3, i = 2, 3, \ldots, p, p \ge 14$. To obtain $GSc(W_p; x)$, we take two cases:

<u>Case 1:</u> If the vertices of $V(W_p)$ are adjacent, then

$$S_d(G,1) = \sum_{i=2}^{p} [degu_1 + degu_i] + \sum_{i=2}^{p-1} [degu_i + degu_{i+1}] + [degu_p + degu_2]$$
$$= (p-1)(p+8).$$

<u>Case 2:</u> If the vertices of $V(W_p)$ are not adjacent, we assume that there are two vertices u and v are not adjacent in $V(W_p)$, then there are distinct two (u, v) – paths Q_1 and Q_2 , the one path Q_1 passes through the vertices which have third degrees and the other path Q_2 passes through the vertex u_1 which have (p-1) degree, (center vertex of a wheel graph).

Let $d^{GS}(u, v; Q_i)$ be the generalized Schultz distance between u and v where u and v are representing the ends of the path Q_i in a wheel graph W_p , for i = 1, 2. From clear that the length of Q_2 is 2, that is, $l(Q_2) = 2$.

If $l(Q_1) = 2$, then the vertices must be consecutive, that is u_i, u_{i+1}, u_{i+2} , for all $i = 2, 3, \ldots, p$, where $u_{p+r} = u_{r+1}$, r = 1, 2. Since, the lowest order of a wheel graph is four, then

 $d^{GS}(u_i, u_{i+2}; Q_1) \leq d^{GS}(u_i, u_{i+2}; Q_2)$ at $l(Q_1) = 2$, for all $i = 2, 3, ..., p, p \geq 4$, where $u_{p+r} = u_{r+1}$, r = 1, 2.

If $l(Q_1) = j$, $3 \le j \le \left\lceil \frac{p-1}{2} \right\rceil$, then the vertices also must to be consecutive, that is $Q_1 = u_i, u_{i+1}, u_{i+2}, \ldots, u_{i+j}$, for all $i = 2, 3, \ldots, p$, where $u_{p+r} = u_{r+1}, r = 1, 2, \ldots, j$.

 $u_i, u_{i+1}, u_{i+2}, \dots, u_{i+j}$, for all $i = 2, 3, \dots, p$, where $u_{p+r} = u_{r+1}$, $r = 1, 2, \dots, j$. Now, we find a relation between j and p when $d^{GS}(u_i, u_{i+j}; Q_1) = d^{GS}(u_i, u_{i+j}; Q_2)$, then

$$\begin{split} \min_{Q_1} \left[\left\{ degu_i + \sum_{w \in V(Q_1) - \{u_i, u_{i+j}\}} degw + degu_{i+j} \right\} l(Q_1) \\ &= \min_{Q_2} \left[\{ degu_i + degu_1 + degu_{i+j} \} l(Q_2) \right] \\ &\Longrightarrow \{3 + 3(j-1) + 3\} (j) = \{3 + p - 1 + 3\} (2) \\ &\Longrightarrow 3j (j+1) = 2(p+5) \\ &\Longrightarrow 3j^2 + 3j - 2(p+5) = 0 \\ &\Longrightarrow j = \frac{1}{6} (-3 + \sqrt{129 + 24p}). \end{split}$$

Since the value j is a positive integer, then we take the greatest integer function of $\frac{1}{6}(-3+\sqrt{129+24p})$, that is, $j = \left\lfloor \frac{-3+\sqrt{129+24p}}{6} \right\rfloor$. If $k \leq j, j \geq 3$, then we have $d^{GS}(u,v;Q_1) \leq d^{GS}(u,v;Q_2)$, then $S_d(W_p,k) = S_d(W_p,l(Q_1)) = (p-1)\sum_{k=3}^j 3(k+1)$, $j = \left\lfloor \frac{-3+\sqrt{129+24p}}{6} \right\rfloor$, $p \geq 14$, where (p-1) is represent the number of the pairs (u,v) such that $d^{GS}(u,v;Q_1) \leq d^{GS}(u,v;Q_2)$. Now, if k > j, then we have $d^{GS}(u,v;Q_1) > d^{GS}(u,v;Q_2)$, hence,

$$S_d(W_p, 2) = \sum_{i=2}^p \{ degu_i + degu_{i+1} + degu_{i+2} \}$$

+ $\frac{1}{2}(p-1)(p-1-(2j+1))\{ degu + degu_1 + degv \}$
= $9(p-1) + \frac{1}{2}(p-1)(p-2(j+1))(p+5)$
= $\frac{1}{2}(p-1)((p-2(j+1))(p+5) + 18), j = \left\lfloor \frac{-3 + \sqrt{129 + 24p}}{6} \right\rfloor, p \ge 14.$

From (2.3), we obtain the following corollary.

Corollary 4.2. Let W_p be a wheel graph of order $p, p \ge 14$, then:

$$GSc (W_p) = p^3 + (3 - 2j)p^2 + (j^3 + 3j^2 - 6j - 12)p - (j^3 + 3j^2 - 8j - 8)$$

where $j = \left[\frac{-3+\sqrt{129+24p}}{6}\right]$.

Theorem 4.3. Let W_p be a wheel graph of order $p, p \ge 15$, then:

$$GSc^* (W_p; x) = 3(p-1)(p+2)x + \frac{9}{2}(p-1)((p-2(j+1))(p-1)+6) x^2 + (p-1)\sum_{k=3}^{j} 3^{k+1}x^k, j = \left\lfloor \frac{W(6(p-1)\log 3)}{\log 3} \right\rfloor.$$

Proof:

Let $V(W_p) = \{u_1, u_2, \dots, u_p\}$, where $degu_1 = p - 1$ and $degu_i = 3, i = 2, 3, \dots, p, p \ge 14$. To obtain $GSc^*(W_p; x)$, we take two cases:

<u>Case 1:</u> If the vertices of $V(W_p)$ are adjacent, then

$$S_d^*(G, 1) = \sum_{i=2}^p [degu_1 \times degu_i] + \sum_{i=2}^{p-1} [degu_i \times degu_{i+1}] + [degu_p \times degu_2]$$

= 3(p-1)(p+2).

<u>Case 2:</u> If the vertices of $V(W_p)$ are not adjacent, we assume that there are two vertices u and v are not adjacent in $V(W_p)$, then there are distinct two (u, v) – paths Q_1 and Q_2 , the one path Q_1 passes through the vertices which have third degrees and the other path Q_2 passes through the vertex u_1 which have (p-1) degree, (center vertex of a wheel graph).

Let $d^{GS^*}(u, v; Q_i)$ be the generalized modified Schultz distance between u and v, where u and v are are representing the ends of the path Q_i in a wheel graph W_p , for i = 1, 2. From clear that the length of Q_2 is 2, that is, $l(Q_2) = 2$.

If $l(Q_1) = 2$, then the vertices must be consecutive, that is u_i, u_{i+1}, u_{i+2} , for all i = 2, 3, ..., p, where $u_{p+r} = u_{r+1}$, r = 1, 2. Since, the lowest order of a wheel graph is four, then

 $d^{GS^*}(u_i, u_{i+2}; Q_1) \le d^{GS^*}(u_i, u_{i+2}; Q_2)$ at $l(Q_1) = 2$, for all $i = 2, 3, ..., p, p \ge 4$, where $u_{p+r} = u_{r+1}$, r = 1, 2.

If $l(Q_1) = j, 3 \le j \le \left\lceil \frac{p-1}{2} \right\rceil$, then the vertices also must to be consecutive, that is $Q_1 = u_i, u_{i+1}, u_{i+2}, \ldots, u_{i+j}$, for all $i = 2, 3, \ldots, p$, where $u_{p+r} = u_{r+1}, r = 1, 2, \ldots, j$.

Now, we find the relation between j and p when $d^{GS^*}(u_i, u_{i+j}; Q_1) = d^{GS^*}(u_i, u_{i+j}; Q_2)$, then

$$\begin{split} \min_{Q_1} \left[\left\{ degu_i \times \prod_{w \in V(Q_1) - \{u_i, u_{i+j}\}} degw \times degu_{i+j} \right\} l(Q_1) \right] \\ &= \min_{Q_2} \left[\{ degu_i \times degu_1 \times degu_{i+j} \} l(Q_2) \right] \\ &\Longrightarrow \left\{ 3 \times 3^{(j-1)} \times 3 \right\} (j) = \{ 3 \times (p-1) \times 3 \} (2) \\ &\implies 3^j j = 6 (p-1) \\ &\implies j e^{\log 3^j} = 6 (p-1) \\ &\implies j \log 3 e^{j \log 3} = 6 (p-1) \log 3. \end{split}$$

By taking the Lambert function [18] to both sides of this equation, we get

$$\implies L_a(jlog3e^{jlog3}) = L_a(6(p-1)log3)$$
$$\implies jlog3 = L_a(6(p-1)log3)$$

$$\implies j = L_a(6(p-1)\log 3)/\log 3$$

Since the value *i* is a positive integer, then we take the greatest integer function of

Since the value *j* is a positive integer, then we have the greatest angle 1 and $L_a(6(p-1)\log 3)/\log 3$, that is, $j = \left\lfloor \frac{L_a(6(p-1)\log 3)}{\log 3} \right\rfloor$. If $k \le j, j \ge 3$, then we have $d^{GS^*}(u, v; Q_1) \le d^{GS^*}(u, v; Q_2)$, then $S_d^*(W_p, k) = S_d^*(W_p, l(Q_1)) = (p-1)\sum_{k=3}^j 3^{(k+1)}, j = \left\lfloor \frac{L_a(6(p-1)\log 3)}{\log 3} \right\rfloor, p \ge 15$, where (p-1) is representing the number of the pairs (u, v) such that $d^{GS^*}(u, v; Q_1) \leq d^{GS^*}(u, v; Q_2)$.

Now, if k > j, then we have $d^{GS^*}(u, v; Q_1) > d^{GS^*}(u, v; Q_2)$, hence,

$$S_d^* (W_p, 2) = \sum_{i=2}^{p} \{ degu_i \times degu_{i+1} \times degu_{i+2} \}$$

+ $\frac{1}{2}(p-1)(p-1-(2j+1)) \{ degu \times degu_1 \times degv \}$
= $27 (p-1) + \frac{1}{2} (p-1) (p-2 (j+1)) (9p-9)$
= $\frac{9}{2}(p-1)((p-2 (j+1))(p-1) + 6), j = \left\lfloor \frac{L_a (6 (p-1) \log 3)}{\log 3} \right\rfloor ., p \ge 15.$

From (2.6), we obtain the following corollary. **Corollary 4.4.** Let W_p be a wheel graph of order $p, p \ge 15$, then:

$$GSc^* (W_p) = \frac{3}{4}(p-1)(6j(3^j-4p+4) - 3^{j+1} + 12p^2 - 32p + 23),$$

where $j = \left\lfloor \frac{L_a(6(p-1)log3)}{log3} \right\rfloor$. **Corollary 4.5.** Let W_p be a wheel graph of order p, then

(i)
$$\overline{GSc}(W_p) = \frac{2(j^3+3j^2-2j(p+4)+p(p+4)-8)}{p}, \ p \ge 14.$$

(ii) $\overline{GSc^*}(W_p) = \frac{3(6j(3^j-4p+4)-3^{j+1}+12p^2-32p+23)}{2p}, \ p \ge 15.$

5 Conclusion

The importance of the generalization of Schultz and modified Schultz distances lies in their ability to determine the least possible sum of all the degrees of vertices (or the product of all the degrees of vertices) multiplied by the length of the path. This benefit is more significant compared to the original Schultz and modified Schultz distances, as it takes into account the influence of all degrees of vertices on the chosen path. This enhanced consideration of vertex degrees allows for a more comprehensive analysis of the graph's properties and contributes to a more accurate understanding of its topological features.

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