The Schultz Index and Schultz Polynomial of the Jahangir Graphs $J_{5,m}$

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Abstract

Let $G$ be simple connected graph with the vertex and edge sets $V(G)$ and $E(G)$, respectively. The Schultz and Modified Schultz indices of a connected graph $G$ are defined as

$$Sc(G) = \frac{1}{2} \sum_{u,v \in V(G)} (d_u + d_v)d(u,v) \quad \text{and} \quad Sc^*(G) = \frac{1}{2} \sum_{u,v \in V(G)} (d_u \times d_v)d(u,v),$$

where $d(u,v)$ is the distance between vertices $u$ and $v$; $d_v$ is the degree of vertex $v$ of $G$. In this paper, computation of the Schultz and Modified Schultz indices of the Jahangir graphs $J_{5,m}$ is proposed.

Keywords

Wiener Index, Schultz Index, Modified Schultz Index, Distance, Jahangir Graphs

1. Introduction

Let $G$ be simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. For vertices $u$ and $v$ in $V(G)$, we denote by $d(u,v)$ the topological distance i.e., the number of edges on the shortest path, joining the two vertices of $G$.

A topological index is a numerical quantity derived in an unambiguous manner from the structure graph of a molecule. As a graph structural invariant, i.e. it does not depend on the labelling or the pictorial representation of a graph. Various topological indices usually reflect molecular size and shape.

As an oldest topological index in chemistry, the Wiener index was first introduced by Harold Wiener [1] in 1947 to study the boiling points of paraffin. It plays an important role in the so-called inverse structure-property relationship problems. The Wiener index of $G$ is defined as [1]-[7]:

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The Hosoya polynomial was introduced by Haruo Hosoya, in 1988 \[8\] and defined as follows:

\[
W(G) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} d(v, u) \]

The number of incident edges at vertex \(v\) is called degree of \(v\) and denoted by \(d_v\).

The Schultz index of a molecular graph \(G\) was introduced by Schultz [9] in 1989 for characterizing alkanes by an integer as follow:

\[
Sc(G) = \frac{1}{2} \sum_{[u,v] \in E(G)} (d_u + d_v) d(u,v). 
\]

The Modified Schultz index of a graph \(G\) was introduced by S. Klavžar and I. Gutman in 1996 as follow [10]:

\[
Sc^*(G) = \frac{1}{2} \sum_{[u,v] \in E(G)} (d_u \times d_v) d(u,v). 
\]

Also the Schultz and Modified Schultz polynomials of \(G\) are defined as:

\[
Sc(G,x) = \frac{1}{2} \sum_{[u,v] \in E(G)} (d_u + d_v) x^{d(u,v)} 
\]

\[
Sc^*(G,x) = \frac{1}{2} \sum_{[u,v] \in E(G)} (d_u \times d_v) x^{d(u,v)} 
\]

where \(d_u\) and \(d_v\) are degrees of vertices \(u\) and \(v\).

The Schultz indices have been shown to be a useful molecular descriptors in the design of molecules with desired properties, reader can see the paper series [11]-[29].

In this paper computation of the Schultz and Modified Schultz indices of the Jahangir graphs \(J_{5,m}\) are proposed. The Jahangir graphs \(J_{5,m}\) \(\forall m \geq 3\) is defined as a graph on \(5m + 1\) vertices and \(6m\) edges i.e., a graph consisting of a cycle \(C_{5m}\) with one additional vertex (Center vertex \(c\)) which is adjacent to \(m\) vertices of \(C_{5m}\) at distance 5 to each other on \(C_{5m}\). Some example of the Jahangir graphs and the general form of this graph are shown in Figure 1 and Figure 2 and the paper series [30]-[35].

**Figure 1.** Some examples of the Jahangir graphs \(J_{5,3}, J_{5,4}, J_{5,5}, J_{5,6}\) and \(J_{5,8}\).
2. Results and Discussion

In this present section, we compute the Schultz and Modified Schultz indices and the Schultz and Modified Schultz polynomials of the Jahangir graphs \( J_{n,m} \) for all integer numbers \( \forall m \geq 3 \) as.

Theorem 1. Let \( J_{5,m} \) be the Jahangir graphs for all integer numbers \( \forall m \geq 3 \). Then, the Schultz, Modified Schultz indices and indices are as:

The Schultz index and polynomial are equal to

\[
Sc(J_{5,m}, x) = \left[ m^2 + 27m \right] x^1 + \left[ 7m^2 + 23m \right] x^2 + \left[ 12m^2 + 16m \right] x^3 \\
+ \left[ 20m^2 - 24m \right] x^4 + \left[ 16m^2 - 24m \right] x^5 + \left[ 8m^2 - 20m \right] x^6,
\]

\[
Sc(J_{5,m}) = 259m^2 - 215m.
\]

The Modified Schultz index and polynomial are equal to:

\[
Sc^*(J_{5,m}, x) = \left[ 3m^2 + 24m \right] x^1 + \left[ 17m^2 + 19m \right] x^2 \left( \frac{2}{2} \right) + \left[ 16m^2 + 12m \right] x^3 \\
+ \left[ 24m^2 - 32m \right] x^4 + \left[ 16m^2 - 24m \right] x^5 + \left[ 8m^2 - 20m \right] x^6,
\]

\[
Sc^*(J_{5,m}) = 292m^2 - 289m.
\]

Proof. Let \( J_{5,m} \) be Jahangir graphs \( \forall m \geq 3 \) with \( 5m + 1 \) vertices and \( 6m \) edges. From Figure 1 and Figure 2, we see that \( 4 \) \( m \) vertices of \( J_{5,m} \) have degree two and \( m \) vertices of \( J_{5,m} \) have degree three and one additional vertex (Center vertex) of \( J_{5,m} \) has degree \( m \). Thus we have three partitions of the vertex set \( V(J_{5,m}) \) as follow

\[
V_2 = \{ v \in V(J_{5,m}) \left| d_v = 2 \right. \} \rightarrow |V_2| = 4m
\]

\[
V_3 = \{ v \in V(J_{5,m}) \left| d_v = 3 \right. \} \rightarrow |V_3| = m
\]

\[
V_m = \{ c \in V(J_{5,m}) \left| d_c = m \right. \} \rightarrow |V_m| = 1
\]

Obviously, \( V(J_{5,m}) = V_2 \cup V_3 \cup V_m \) and \( V_2 \cap V_3 \cap V_m = \emptyset \), thus

\[
|E(J_{5,m})| = \frac{1}{2} \left[ 2 \times |V_2| + 3 \times |V_3| + m \times |V_m| \right] = 6m.
\]

Now, for compute the Schultz and Modified Schultz indices and the Schultz and Modified Schultz polynomials of the Jahangir graphs \( J_{n,m} \), we see that for all vertices \( u, v \) in \( V(J_{5,m}) \), \( \exists d(u,v) \in \{1, 2, \cdots, 6\} \) and the diameter of the Jahangir graph \( J_{5,m} \) is equal to \( d(J_{5,m}) = 6 \).

Now, we compute all cases of \( d(u,v) \)-edge-paths \( d(u,v) = 1, 2, \cdots, 6 \) of \( J_{5,m} \) in Table 1.
Table 1. All cases of $d(u,v)$-edge-paths $d(u,v) = 1, 2, \ldots, 6$ of the Jahangir graph $J_{5,m}$.

<table>
<thead>
<tr>
<th>The distance $d(u,v) = i$</th>
<th>degrees of $d_u$ &amp; $d_v$</th>
<th>Number of $i$-edges paths</th>
<th>Term of Schultz polynomial</th>
<th>Term of Modified Schultz polynomial</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2 &amp; 2</td>
<td>$3m = 2</td>
<td>V_i</td>
<td>-</td>
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<tr>
<td>1</td>
<td>2 &amp; 3</td>
<td>$2m = 2</td>
<td>V_i</td>
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<tr>
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<td>3 &amp; 3</td>
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<td>0</td>
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<td>1</td>
<td>2 &amp; m</td>
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<td>V_i</td>
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<tr>
<td>2</td>
<td>3 &amp; 3</td>
<td>$\frac{1}{2}</td>
<td>V_i</td>
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<tr>
<td>2</td>
<td>2 &amp; m</td>
<td>$2m = 2</td>
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<td>$2m + \frac{1}{2}</td>
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<td>0</td>
</tr>
<tr>
<td>6</td>
<td>2 &amp; 2</td>
<td>$\frac{1}{2}</td>
<td>V_i</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>2 &amp; 3</td>
<td>0</td>
<td>0</td>
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<tr>
<td>6</td>
<td>3 &amp; m</td>
<td>0</td>
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</tr>
</tbody>
</table>
For example, in case \( d(u,v) = 1, \forall v, u \in V(J_{5,m}) \); one can see that there are \( |V_j| = m \) 1-edges paths between the vertex \( c \) and vertices from \( V_j \) (where \( d_c + d_v = m + 3, d_c \times d_v = 3m \)). There exist two 1-edges paths starts every vertex \( u \in V_j \) until \( v \in V_j \) (where \( d_u + d_v = 5, d_u \times d_v = 6 \)). There are 3 \( m \) 1-edges paths between two vertices \( u, v \in V_j \subset V(J_{5,m}) \) (two adjacent vertices or edges), such that \( d_u + d_v = d_u \times d_v = 4 \). Thus, the first terms of the Schultz and Modified Schultz polynomials of \( J_{5,m} \) are equal to
\[
(12m + 10m + (m + 3)m)x^1 = (m^2 + 27m)x^1 \text{ and } (12m + 12m + 3m^2)x = (3m^2 + 24m)x \text{ respectively.}
\]

Also, in case \( d(u,v) = 2, \forall v, u \in V(J_{5,m}) \); there are two 2-edges paths between Center vertex \( c \in V(J_{5,m}) \) and other vertices of vertex set \( V_j \subset V(J_{5,m}) \). \( \frac{1}{2}|V_j| = (m-1) \) 2-edges paths between all vertices of \( u, v \in V_j \subset V(J_{5,m}) \) and \( 2|V_j| = 2 \) 2-edges paths start from vertices of \( V_j \) until vertices of \( V_j \) and \( V_2 \subset V(J_{5,m}) \). Thus, the second terms of the Schultz and Modified Schultz polynomials of \( J_{5,m} \) are equal to
\[
(12m + 10m + 3m(m - 1) + 2m(m + 2))x^2 \text{ and } (12m + 12m + m(m - 1) + 4m^2)x^2 \text{ respectively.}
\]
By using the definition of the Jahangir graphs and Figure 1 and Figure 2, we can compute other terms of the Schultz and Modified Schultz polynomials of \( J_{5,m} \). We compute and present all necessary results on based the degrees of \( d_u \) & \( d_v \) for all cases of \( d(u,v) \)-edge-paths \( d(u,v) = 1, 2, \cdots, 6 \) in following table.

Now, we can compute all coefficients of the Schultz \( Sc(J_{5,m}, x) \) and Modified Schultz \( Sc'(J_{5,m}, x) \) polynomials and indices of \( J_{5,m} \) by using all cases of the \( d(u,v) \)-edge-paths \( d(u,v) = 1, 2, \cdots, 6 \) of the Jahangir graph \( J_{5,m} \) in Table 1 and alternatively

\[
Sc(J_{5,m}, x) = \frac{1}{2} \sum_{u,v \in V(J_{5,m})} (d_u + d_v) x^{d(u,v)} = \left[ 12m + 12m + 0 + 0 + m(m+3) \right] x^1
\]
\[
+ \left[ 12m + 10m + 3(m(m-1) + 2m(m+2)) + 0 \right] x^2
\]
\[
+ \left[ 8m(m-1) + 10m(m-2) + 0 + 2m(m+2) + 0 \right] x^3
\]
\[
+ \left[ 8m(2m-3) \right] x^4
\]
\[
+ \left[ 4m(2m-5) \right] x^5
\]
\[
= \left[ m^2 + 27m \right] x^1 + \left[ 7m^2 + 23m \right] x^2 + \left[ 12m^2 + 16m \right] x^3 + \left[ 20m^2 - 24m \right] x^4
\]
\[
+ \left[ 16m^2 - 24m \right] x^5 + \left[ 8m^2 - 20m \right] x^6.
\]

From the definition of Schultz index and the Schultz Polynomial of \( G \), we can compute the Schultz index of the Jahangir graph \( J_{5,m} \) by the first derivative of Schultz polynomial of \( J_{5,m} \) (evaluated at \( x = 1 \)) as follow:

\[
Sc(J_{5,m}) = \frac{\partial Sc(J_{5,m}, x)}{\partial x} \bigg|_{x=1} = \frac{\partial}{\partial x} \left( m^2 + 27m \right) x + \left( 7m^2 + 23m \right) x^2 + \left( 12m^2 + 16m \right) x^3
\]
\[
+ \left( 20m^2 - 24m \right) x^4 + \left( 16m^2 - 24m \right) x^5 + \left( 8m^2 - 20m \right) x^6 \bigg|_{x=1}
\]
\[
= \left[ m^2 + 27m \right] x + \left[ 7m^2 + 23m \right] x^2 + \left[ 12m^2 + 16m \right] x^3 + \left[ 20m^2 - 24m \right] x^4
\]
\[
+ \left[ 16m^2 - 24m \right] x^5 + \left[ 8m^2 - 20m \right] x^6 \bigg|_{x=1}
\]
\[
= 259m^2 - 215m.
\]

And also Modified Schultz polynomial of \( J_{5,m} \) is equal to

\[
Sc'(J_{5,m}, x) = \frac{1}{2} \sum_{u,v \in V(J_{5,m})} (d_u \times d_v) x^{d(u,v)} = \left[ 12m + 12m + 0 + 0 + 3m^2 \right] x^1
\]
\[
+ \left[ 12m + 12m + m(m-1) + 4m^2 + 0 \right] x^2
\]
\[
+ \left[ 8m(m-1) + 12m(m-2) + 0 + 4m^2 + 0 \right] x^3
\]
\[
+ \left[ 8m(2m-3) \right] x^4
\]
\[
+ \left[ 4m(2m-5) \right] x^5
\]
\[
= \left[ 3m^2 + 24m \right] x^1 + \left[ \frac{17}{2} m^2 + \frac{19}{2} m \right] x^2 + \left[ 16m^2 + 12m \right] x^3 + \left[ 24m^2 - 32m \right] x^4
\]
\[
+ \left[ 16m^2 - 24m \right] x^5 + \left[ 8m^2 - 20m \right] x^6.
\]
And from the first derivative of Schultz Modified polynomial of the Jahangir graph $J_{5,m}$ (evaluated at $x = 1$), the Modified Schultz index of $J_{5,m}$ is equal to:

$$Sc^*(J_{5,m}) = \left. \frac{\partial Sc^*(J_{5,m}, x)}{\partial x} \right|_{x=1}$$

$$= \frac{\partial}{\partial x} \left(3m^2 + 24m)x^2 + (m^2 + m)x^2 + (16m^2 + 12m)x^3 + (24m^2 - 32m)x^4 + (16m^2 - 24m)x^5 + (8m^2 - 20m)x^6 \right)_{x=1}$$

$$= 292m^2 - 289m.$$

Here these completed the proof of Theorem 1. ■

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Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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