Leap Zagreb coindex and Wiener polarity index of Jahangir graphs

Raad Sehen Haoer\(^a,^*\)

\(^a\)Open Educational College, Ministry of Education, Department of Mathematics, Al-Qadisiya Centre, Iraq.

Abstract

The Leap Zagreb coindices and the Wiener polarity index are examples of less frequently studied topological indices that are based on the number of vertices lying at second and third distances from a given vertex. These indices have applications in QSAR and QSPR studies. In this paper, we obtain leap Zagreb coindices and the Wiener polarity index of a rotationally symmetric subfamily of circulant graphs known as Jahangir graphs.

Keywords: Topological indices, leap Zagreb index, Jahangir graphs.

1. Introduction

Let \(\Gamma\) denote a simple connected graph with vertex set \(V\) and edge set \(E\). The distance \(d_\Gamma(v, w)\) between two vertices \(v, w \in V(\Gamma)\) is the length of a path of minimal length joining \(v\) with \(w\) in \(\Gamma\). Let \(u, x, y \in V(\Gamma)\) and \(e = xy \in E(\Gamma)\). The number of vertices lying at distance \(k\) from a vertex \(v \in V(\Gamma)\) is called the \(k\)-th degree \(d(v|k)\) of the vertex \(v\).

The Zagreb indices were first introduced in [1] where the authors examined the dependence of total \(\pi\)-electron energy of molecular structures. For a molecular graph \(\Gamma\), the first Zagreb index \(M_1(\Gamma)\) and the second Zagreb index \(M_2(\Gamma)\) are defined, respectively, as follows.

\[
M_1(\Gamma) = \sum_{v \in V(\Gamma)} d_\Gamma(v)^2 = \sum_{uv \in E(\Gamma)} (d_\Gamma(u) + d_\Gamma(v))
\]

\[
M_2(\Gamma) = \sum_{uv \in E(\Gamma)} d_\Gamma(u)d_\Gamma(v).
\]

\(^*\)Corresponding author

Email address: raadsehen@gmail.com (Raad Sehen Haoer)

Received: 5 January 2021; Accepted: 28 May 2021; Published Online: 29 July 2021.
The Zagreb coindices were defined as the modification of the Zagreb index by Ashrafi et al. [2] as follows.
\[
\overline{M}_1(\Gamma) = \sum_{uv \notin E(\Gamma)} (d_\Gamma(u) + d_\Gamma(v))
\]
\[
\overline{M}_2(\Gamma) = \sum_{uv \notin E(\Gamma)} d_\Gamma(u)d_\Gamma(v).
\]

Modifications of the Zagreb indices based on the second neighbors of the vertices of a graph were defined by Gutman et al. [3]. These indices are called the first leap Zagreb indices, second leap Zagreb indices and third leap Zagreb indices respectively, are defined as follows.
\[
LM_1(\Gamma) = \sum_{v \in V(\Gamma)} d_\Gamma^2(v \mid 2)
\]
\[
LM_2(\Gamma) = \sum_{uv \in E(\Gamma)} d_\Gamma(u \mid 2)d_\Gamma(v \mid 2)
\]
\[
LM_3(\Gamma) = \sum_{v \in V(\Gamma)} d_\Gamma(v \mid 1)d_\Gamma(v \mid 2) = \sum_{uv \in E(\Gamma)} (d_\Gamma(u \mid 2) + d_\Gamma(v \mid 2)).
\]

It can be seen that the coindices of the second and third version of leap Zagreb indices can be established as follows.
\[
\overline{LM}_2(\Gamma) = \sum_{uv \notin E(\Gamma)} d_\Gamma(u \mid 2)d_\Gamma(v \mid 2)
\]
\[
\overline{LM}_3(\Gamma) = \sum_{uv \notin E(\Gamma)} (d_\Gamma(u \mid 2) + d_\Gamma(v \mid 2)).
\]

Wiener [4] introduced another topological invariant of a graph \(\Gamma\) known as Wiener polarity index \(W_p(\Gamma)\). It is defined as the number of unordered pairs of vertices \(\{u, v\} \subseteq V(\Gamma)\) which are at distance 3 in \(\Gamma\). Mathematically, \(W_p(\Gamma)\) is defined in the following equation along with an equivalent and comparatively easy representation.
\[
W_p(\Gamma) = \left| \{\{u, v\} \subseteq V(\Gamma) \mid d_\Gamma(u, v) = 3\} \right| = \frac{1}{2} \sum_{v \in V(\Gamma)} d_\Gamma(v \mid 3).
\]

Wiener polarity index has attracted the attention of a remarkably large number of mathematicians. Hosoya [5] found a physical-chemical interpretation of \(W_p(\Gamma)\). The Wiener polarity index of fullerenes and hexagonal systems was studied in [6]. The Wiener polarity index of square, hexagonal and triangular lattices were studied in [7]. Recently, Arockiaraj et al. [8] studied the hyper-Wiener and Wiener polarity indices of silicate and oxide networks. Authors in [9, 10] and [11] studied some degree and distance based indices of product graphs and nanotubes. In [12, 13, 14, 15], authors studied some newly defined degree based topological indices of some important families of graphs. Also, Liu and Liu [16] studied the Wiener polarity index of dendrimers. For a survey of results on Wiener index, Wiener polarity index and some other variations of Wiener index, see [17]. Topological indices have been extensively studied for their applications in QSAP and QSPR studies, see [18, 19, 20, 21]. More on the applications of topological indices can be found in [22, 23, 24, 25, 26, 27, 28]. The study of topological indices for several types of graphs have been carried out in the literature, for example see [2, 29]. Several degree and distance-based topological indices of Jahangir graphs are studied in [30, 31, 32].

In this paper we study leap Zagreb coindices and the Wiener polarity index of Jahangir graphs \(J_{n,m}\).

2. Jahangir graphs

The Jahangir graph \(J_{n,m}\) is a graph with \(nm + 1\) number of vertices and \(m(n + 1)\) number of edges for all \(n \geq 2\) and \(m \geq 3\). The Jahangir graph \(J_{n,m}\) consists of a cycle \(C_{mn}\) and a single vertex that is adjacent to \(m\) vertices of the cycle that are at distance \(n\) from each other. The Jahangir graphs \(J_{6,4}\) is shown in Figure 1.
3. First, second and third degrees of vertices in Jahangir graphs $J_{n,m}$

In the following lemma, we present some structural properties of the Jahangir graphs $J_{n,m}$.

**Lemma 3.1.** Let $J_{n,m}$ denote the Jahangir graphs (see Figure 1). Then the first, second and third degrees of vertices in $J_{n,m}$ are given by the following expressions.

(a) $d_\Gamma(y|1) = \begin{cases} 
  m, & \text{if } y = v, \\
  3, & \text{if } y = u, \\
  2, & \text{otherwise, where } n \geq 3, m \geq 4.
\end{cases}$

(b) $d_\Gamma(y|2) = \begin{cases} 
  2m, & \text{if } y = v, \\
  m + 1, & \text{if } y = u, \\
  3, & \text{if } y = w, \\
  2, & \text{otherwise, where } n \geq 4, m \geq 4.
\end{cases}$

(c) $d_\Gamma(y|3) = \begin{cases} 
  2m, & \text{if } y = v, \\
  2m - 2, & \text{if } y = u, \\
  m + 1, & \text{if } y = w, \\
  3, & \text{if } y = x', \\
  2, & \text{otherwise, where } n \geq 5, m \geq 4.
\end{cases}$

The computation of coindices of a graph requires information about the edge set of complement of the given graph. Let $E$ and $\overline{E}$ respectively denote the edge set of the Jahangir graph and edge set of the complement of the Jahangir graph $J_{n,m}$, that is, $E = E(J_{n,m})$ and $\overline{E} = E(\overline{J}_{n,m})$. Then the edge partition of the edge set of Jahangir graph can be presented by the Table 1.

In Table 2 we give the edge partition of the complement of Jahangir graph with respect to the type of its vertices.

4. Leap Zagreb coindices of Jahangir graphs $J_{n,m}$

Now we proceed towards the main calculations of the indices of Jahangir graphs $J_{n,m}$. First we calculate the three leap Zagreb coindices of the graphs $J_{n,m}$.
Table 1: The edge partition of the graph $J_{n,m}$.

<table>
<thead>
<tr>
<th>$E$</th>
<th>$u$</th>
<th>$v$</th>
<th>$w$</th>
<th>$x$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u$</td>
<td>0</td>
<td>$m$</td>
<td>2$m$</td>
<td>0</td>
</tr>
<tr>
<td>$v$</td>
<td>$m$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$w$</td>
<td>2$m$</td>
<td>0</td>
<td>0</td>
<td>2$m$</td>
</tr>
<tr>
<td>$x$</td>
<td>0</td>
<td>0</td>
<td>2$m$</td>
<td>$m(n-4)$</td>
</tr>
</tbody>
</table>

Table 2: The edge partition of the graph $J_{n,m}$.

<table>
<thead>
<tr>
<th>$E$</th>
<th>$u$</th>
<th>$v$</th>
<th>$w$</th>
<th>$x$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u$</td>
<td>$\frac{m(m-1)}{2}$</td>
<td>0</td>
<td>$m(2m-2)$</td>
<td>$m^2(n-3)$</td>
</tr>
<tr>
<td>$v$</td>
<td>0</td>
<td>0</td>
<td>$2m$</td>
<td>$m(n-3)$</td>
</tr>
<tr>
<td>$w$</td>
<td>$m(2m-2)$</td>
<td>$2m$</td>
<td>$2m[2m-1]$</td>
<td>$2m[m(n-3)-1]$</td>
</tr>
<tr>
<td>$x$</td>
<td>$m^2(n-3)$</td>
<td>$m(n-3)$</td>
<td>$2m[m(n-3)-1]$</td>
<td>$\left(\frac{m(n-3)[m(n-3)-1]}{2} - m(n-4)\right)$</td>
</tr>
</tbody>
</table>

**Theorem 4.1.** Then second leap Zagreb coindex of the Jahangir graph $J_{n,m}$ is given by

$$LM_2(J_{n,m}) = \frac{1}{2}(1/2)m^4 + (1/2)m^3 - (13/2)m^2 - (35/2)m + 2m^3n + 6m^2n + 2m^2n^2 - 3mn.$$ 

**Proof.** We use Lemma 3.1 in the definition of second leap Zagreb coindex to simplify the results as follows.

$$LM_2(J_{n,m}) = \sum_{xy \in E(J_{n,m})} d_{J_{n,m}}(x|2) d_{J_{n,m}}(y|2)$$

$$= d(u|2)d(u|2) \left( \frac{m(m-1)}{2} \right) + d(u|2)d(w|2)m(2m-2)$$

$$+ d(w|2)d(x|2)m^2(n-3) + d(w|2)d(v|2)2m + d(w|2)d(w|2) \left( \frac{2m(2m-1)}{2} \right)$$

$$+ d(w|2)d(x|2)2m[m(n-3)-1] + d(x|2)d(v|2)m(n-3)$$

$$+ d(x|2)d(x|2) \left( \frac{m(n-3)[m(n-3)-1]}{2} - m(n-4) \right)$$

$$= (m+1)(m+1) \frac{m(m-1)}{2} + (m+1)(3)m(2m-2)$$

$$+ (m+1)(2m)(n-3) + (3)(2m)2m$$

$$+ (3)(3) \frac{2m(2m-1)}{2} + (3)(2m)[m(n-3)-1]$$

$$+ (2)(2m)m(n-3) + (2)(2) \left( \frac{m(n-3)[m(n-3)-1]}{2} - mn - 4m \right)$$

$$= \frac{m(m-1)(m+1)^2}{2} + 3m(m+1)(2m-2) + 2m^2(m+1)(n-3) + 12m^2$$

$$+ 9m(2m-1) + 12m[m(n-3)-1] + 4m^2(n-3)$$

$$+ 2m(n-3)[m(n-3)-1] - mn + 4m$$

$$= (1/2)m^4 + (1/2)m^3 - (13/2)m^2 - (35/2)m + 2m^3n + 6m^2n + 2m^2n^2 - 3mn.$$ 

This completes the proof.

**Theorem 4.2.** Then third leap Zagreb coindex of the Jahangir graph $J_{n,m}$ is given by

$$LM_3(J_{n,m}) = m^3n + 2m^2n^2 + 3m^2n - 5m^2 - 4mn - 3m.$$
This completes the proof.

Proof. We use Lemma 3.1 in the definition of third leap Zagreb coindex to simplify the results as follows.

\[
\overline{LM}_3(J_{n,m}) = \sum_{xy \notin E(J_{n,m})} (d_{J_{n,m}}(x|2) + d_{J_{n,m}}(y|2))
\]

\[
= (d(u|2) + d(w|2)) \left( \frac{m(m - 1)}{2} \right) + (d(u|2) + d(w|2))m(2m - 2)
\]

\[
+ (d(w|2)(2m(2m - 1))
\]

\[
+ (d(w|2)(2m(2m - 1))m(2m - 2) + (d(u|2) + d(w|2))m(2m - 2)
\]

\[
+ (d(u|2) + d(w|2))m(2m - 2) + (d(u|2) + d(w|2))m(2m - 2)
\]

\[
+ (d(w|2)(2m(2m - 1))m(2m - 2) + (d(u|2) + d(w|2))m(2m - 2)
\]

\[
= (m + 1)(m + 1)\frac{m(m - 1)}{2} + (m + 1)(m + 1)\frac{m(m - 1)}{2}
\]

\[
+ ((m + 1)(2)m(2m - 1) + ((m + 1)(2)m(2m - 1))2m
\]

\[
+ ((m + 1)(2)m(2m - 1) + ((m + 1)(2)m(2m - 1))2m
\]

\[
+ ((m + 1)(2)m(2m - 1) + ((m + 1)(2)m(2m - 1))2m
\]

\[
= m(m + 1)(m + 1) + 2m(m + 4)(m - 1)
\]

\[
+ m^2(m + 3)(n - 3) + 2m(2m + 3)
\]

\[
+ 12m(2m - 1) + 10m(m - 3) - 1]
\]

\[
+ 2m(m + 1)(n - 3) + 2m(n - 3)[m(n - 3) - 1] - mn + 4m
\]

\[
= m^3n + 2m^2n^2 + 3m^2n - 5m^2 - 4mn - 3m.
\]

This completes the proof.

\[\square\]

Theorem 4.3. Then Wiener polarity index of the Jahangir graph \(J_{n,m}\) is given by

\[
W_p(J_{n,m}) = \frac{1}{2}(4m^2 + 3nm - 7m).
\]

Proof. We use Lemma 3.1 in the definition of Wiener polarity index to simplify the results as follows.

\[
W_p(J_{n,m}) = \sum_{x \in \Gamma(J)} \frac{1}{2}d_{\Gamma}(x|3)
\]

\[
= \frac{1}{2}(2m + (2m - 2)m + (m + 1)2m + (3)(n - 3)m)
\]

\[
= \frac{1}{2}(4m^2 + 3nm - 7m).
\]

This completes the proof.

\[\square\]

5. Conclusion and discussion

The pairwise comparisons of the 3D surfaces of the second and third kind of leap Zagreb coindices \(\overline{LM}_1\) and \(\overline{LM}_2\) and the Wiener polarity index of the Jahangir graphs \(J_{n,m}\) is provided in Figure 2.

The Jahangir graphs \(J_{n,m}\) is an infinite family of cycle-based graphs that form a subclass of circulant graphs as well. These are rotationally symmetric graphs. In this paper, we obtain leap Zagreb coindices of these graphs and the Wiener polarity index of Jahangir graphs \(J_{n,m}\).
Figure 2: The comparison between the graphs of $LM_1$ verses $LM_2$ (Left), $LM_2$ verses $W_p$ (Middle) and $LM_1$ verses $W_p$.

References


