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On distance-based topological invariants of Isaac graphs

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Abstract.
Let G be a simple connected graph. The Wiener index of G is the sum of the distances between all unordered pairs of vertices in G. In this paper we derive formulas for the Wiener index and two other Wiener-types such as Schultz and hyper-Wiener indices in the class of chemical compounds whose hydrogen-suppressed molecular graphs are isomorphic to an Isaac graph.

1 Introduction

The Isaac graph J_m, for $m \geq 3$, is the graph consisting of m “segments" isomorphic to the claw $K_{1,3}$ arranged into a cycle, where the leaves of a given segment are connected to the leaves of the preceding and the succeeding segments in the manner indicated in Figure 1: the given segment is plain while the preceding and the succeeding segments are dashed [2, 7].

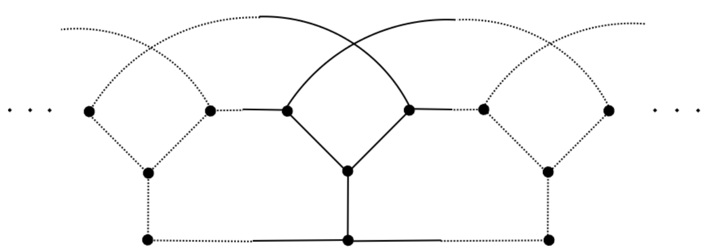

Figure 1. Isaac graphs.

Definition 1.1 (Isaac graph). For each integer $m \geq 3$, the Isaac graph, denoted by J_m, is a simple graph $G = (V, E)$ where

$$\begin{aligned} V &= \{v_{ijk,l} \ : \ i,j,k \in \{0,1\}, 2 \leq i+j+k \text{ and } l \in \{1,2,\ldots,m\}\} \text{ and} \\ E &= \Big\{\{v_{ijk,l}, v_{pqr,s}\} \subseteq V \ : \ \text{either } [i+j+k+p+q+r = 5 \text{ and } l = s] \\ &\qquad \text{or } [(i,j,k) = (p,q,r),\, i+j+k = 2 \text{ and } |l-s| \in \{1, m-1\}]\Big\}. \end{aligned}$$

The Isaac graphs J_4 and J_5 are shown in Figure 2.

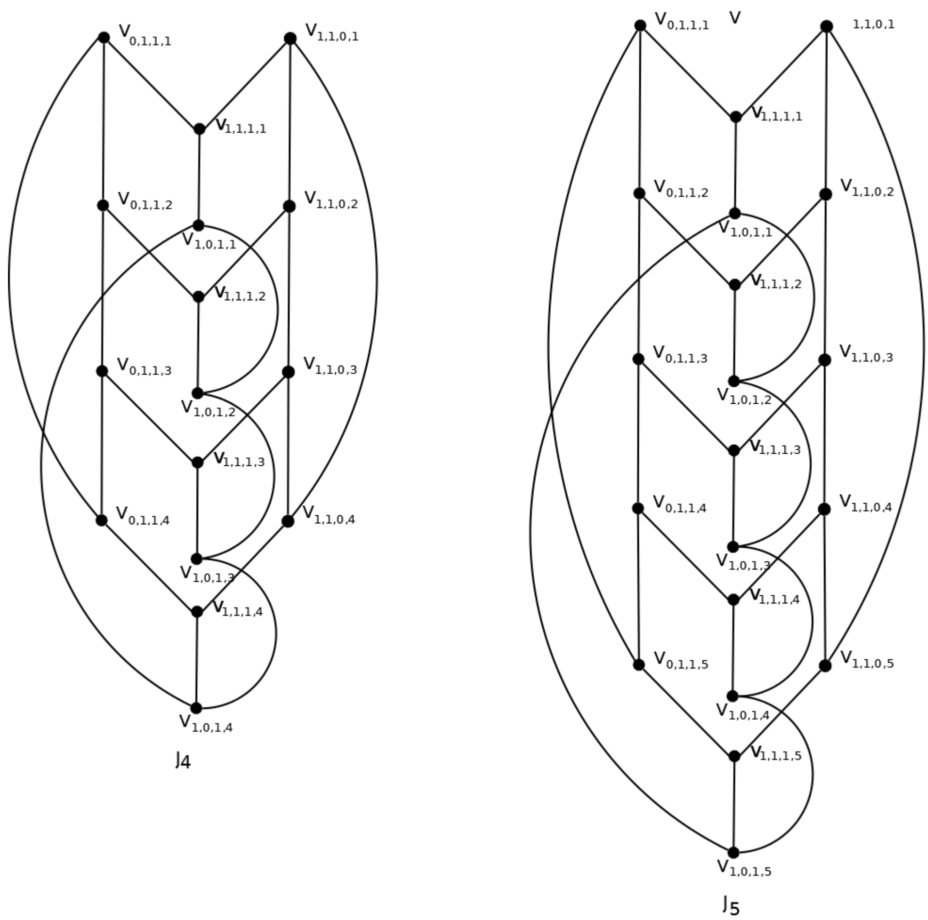

Figure 2. The Isaac graphs J_4 and J_5.

Isaac graphs are isomorphic to hydrogen-suppressed molecular graphs. The invariants considered in this note and applied to Isaac graphs have applications in mathematical chemistry. Poojary et al. [4] computed certain topological indices and polynomials for Isaac graphs. In this paper, we consider Isaac graphs as growing network systems, and the invariants obtained behave uniformly along with an increase in the number of their segments. The formulas obtained for the invariants are easy to use, can easily predict the number of segments needed to reach a given potential value.

The organization of the paper is as follows. Section 2 introduces Isaac graphs along with a constructive definition. Section 3 recalls the necessary background on the Wiener index, and gives a characterization of Isaac graphs in terms of Wiener index. Section 4 gives the definition of the Schultz index and a characterization of Isaac graphs in terms of Schultz index. Section 5 recalls the hyper-Wiener index and gives a characterization of Isaac graphs in terms of hyper-Wiener index.

2 Wiener index of Isaac graphs

The Wiener index is the first topological index defined by the H. Wiener in 1947. He used the distances in the molecular graphs of alkanes to calculate their boiling points [12]. The Wiener index $W(G)$ of a connected graph G is defined as the sum of the distances between all unordered pairs of vertices, i.e.,

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

where $d(u, v)$ is the usual distance, i.e., the minimum length of a path from u to v in G.

The Wiener index was extensively studied in both theoretical and chemical literature. This was due to its correlation with a large number of physicochemical properties of organic molecules and their interesting mathematical properties [6, 9, 10]. Of particular interest are relations between the Wiener index and other distance-based graph invariants. For instance, paper [5] explores the relationship between eccentricities by proving a sharp lower bound on the Wiener index of a tree with a given eccentric sequence.

We start with a straightforward lemma which follows from the structure of J_m, see Figures 1, 2 and 3.

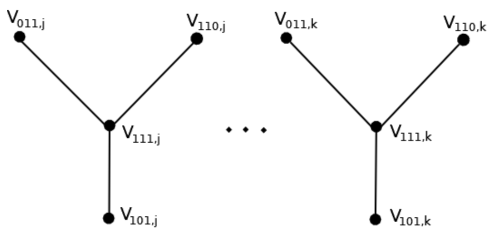

Figure 3. Segments of J_m

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Lemma 2.1. *For any j, k such that $1 \le j, k \le m$, and $|k-j| \le \lfloor \frac{m}{2} \rfloor$, we have*

$$\begin{array}{lllllll} d(v_{011,j}, v_{011,k}) & = & d(v_{101,j}, v_{101,k}) & = & d(v_{110,j}, v_{110,k}) & = & |k-j|, \\ d(v_{111,j}, v_{011,k}) & = & d(v_{111,j}, v_{101,k}) & = & d(v_{111,j}, v_{110,k}) & = & |k-j|+1, \\ d(v_{111,j}, v_{111,k}) & = & d(v_{011,j}, v_{101,k}) & = & d(v_{011,j}, v_{110,k}) & = & d(v_{101,j}, v_{110,k}) = |k-j|+2. \end{array}$$

For any j, k such that $1 \le j, k \le m$, and $|k-j| > \lfloor \frac{m}{2} \rfloor$, we have

$$\begin{array}{lllllll} d(v_{011,j}, v_{011,k}) & = & d(v_{101,j}, v_{101,k}) & = & d(v_{110,j}, v_{110,k}) & = & m-|k-j|, \\ d(v_{111,j}, v_{011,k}) & = & d(v_{111,j}, v_{101,k}) & = & d(v_{111,j}, v_{110,k}) & = & m-|k-j|+1, \\ d(v_{111,j}, v_{111,k}) & = & d(v_{011,j}, v_{101,k}) & = & d(v_{011,j}, v_{110,k}) & = & d(v_{101,j}, v_{110,k}) = m-|k-j|+2. \end{array}$$

Proof. By construction the first segment is adjacent to the last segment in the sense that

$$\{v_{011,1}, v_{011,m}\},\ \{v_{101,1}, v_{101,m}\},\ \{v_{110,1}, v_{110,m}\}$$

are all edges of J_m. This is the reason that justifies the case distinctions in the lemma. □

Our first main theorem reads as follows:

Theorem 2.2. *The Wiener index of the Isaac graph J_m is given by*

$$W(J_m) = \begin{cases} m(2m^2+10m-1) & \text{if } \ m \text{ is even,} \\ m(2m^2+10m-3) & \text{if } \ m \text{ is odd.} \end{cases}$$

Proof. We consider distances between vertices within the same segment, and distances between vertices of distinct segments of J_m. Since every segment is $K_{1,3}$, this gives us

$$\begin{aligned} W(J_m) = mW(K_{1,3}) & \\ + \sum_{1\le j<k\le m} \Big[& d(v_{111,j}, v_{111,k}) + d(v_{111,j}, v_{011,k}) + d(v_{111,j}, v_{101,k}) + d(v_{111,j}, v_{110,k}) \\ & + d(v_{011,j}, v_{111,k}) + d(v_{011,j}, v_{011,k}) + d(v_{011,j}, v_{101,k}) + d(v_{011,j}, v_{110,k})) \\ & + d(v_{101,j} + v_{111,k}) + d(v_{101,j}, v_{110,k}) + d(v_{101,j}, v_{101,k}) + d(v_{101,j}, v_{110,k}) \\ & + d(v_{110,j}, v_{111,k}) + d(v_{110,j}, v_{011,k}) + d(v_{110,j}, v_{101,k}) + d(v_{110,j}, v_{110,k}) \Big]. \end{aligned}$$

Note that $W(K_{1,3}) = 9$. Using the case distinctions in Lemma 2.1, we obtain

$$\begin{aligned} W(J_m) &= 9m + \sum_{\substack{1\le j<k\le m \\ k-j\le \lfloor \frac{m}{2} \rfloor}} (16(k-j)+20) + \sum_{\substack{1\le j<k\le m \\ k-j> \lfloor \frac{m}{2} \rfloor}} (16(m-k+j)+20) \\ &= 9m + 20\binom{m}{2} + 16 \sum_{\substack{1\le j<k\le m \\ k-j\le \lfloor \frac{m}{2} \rfloor}} (k-j) + 16 \sum_{\substack{1\le j<k\le m \\ k-j> \lfloor \frac{m}{2} \rfloor}} (m-k+j)\,. \end{aligned} \tag{2.1}$$

On the other hand, it is easy to show that

$$\sum_{\substack{1\le j<k\le m \\ k-j\le \lfloor \frac{m}{2} \rfloor}} k-j = \begin{cases} \frac{1}{24}m(m+2)(2m-1) & \text{if m is even,} \\ \frac{1}{12}m(m-1)(m+1) & \text{if m is odd,} \end{cases}$$

and that

$$\sum_{\substack{1\le j<k\le m \\ k-j> \lfloor \frac{m}{2} \rfloor}} m-k+j = \begin{cases} \frac{1}{24}m(m-1)(m-2) & \text{if m is even,} \\ \frac{1}{24}m(m-1)(m+1) & \text{if m is odd.} \end{cases}$$

Substituting the above identities into Equation 2.1, we get

$$W(J_m) = \begin{cases} m(2m^2+10m-1) & \text{if m is even}\,, \\ m(2m^2+10m-3) & \text{if m is odd}\,, \end{cases}$$

after some calculations. This completes the proof of the theorem. □

A large number of topological indices were conceived for the purpose of describing relationships between structural formulas and molecular graphs, and many of the distance-based topological indices are variants or generalisations of the Wiener index; see [3] and the recent survey [13] for more information on these indices and chemical applications.

3 Schultz index of Isaac graphs

The Schultz index is another important topological index. The ordinary (vertex) molecular topological index (MTI) of a molecular graph was introduced by Schultz [11] in 1989 and it was eventually named Schultz index, defined as

$$S(G) = \sum_{\{u,v\}\in V(G)} (\deg u + \deg v)d(u,v).$$

Dankelmann and Dossou-Olory [5] characterized a tree that minimizes the Schultz index and the Gutman index among all trees with a given eccentric sequence.

Since J_m is 3 regular, we have $Sc(J_m) = 6W(J_m)$.

Theorem 3.1. *The Schultz index of the Isaac graph J_m is given by*

$$Sc(J_m) = \begin{cases} 6m(2m^2+10m-3) & \textit{if m is odd,} \\ 6m(2m^2+10m-1) & \textit{if m is even.} \end{cases}$$

4 Hyper-Wiener index of Isaac graphs

The hyper-Wiener index of acyclic graphs was introduced by M. Randic in 1993. Later Klein et al. [8] gave generalized hyper-Wiener index for all connected graphs. The hyper-Wiener index $HW(G)$ of a connected graph G is defined as

$$HW(G) = \sum_{\{u,v\}\subseteq V(G)} \binom{1+d(u,v)}{2}.$$

Theorem 4.1. *The hyper Wiener index of J_m is given by*

$$HW(J_m) = \begin{cases} \frac{m}{3}(2m^3 + 21m^2 + 85m - 9) & \text{if } m \text{ even,} \\ \frac{m}{3}(2m^3 + 21m^2 + 79m - 30) & \text{if } m \text{ odd.} \end{cases}$$

Proof. We rewrite $HW(G)$ as

$$HW(J_m) = W(J_m) + \sum_{\{u,v\} \subseteq V(J_m)} d(u,v)^2.$$

Then we consider distances between vertices within the same segment, and distances between vertices of distinct segments of J_m and use the cases distinction in Lemma 2.1. This gives us

$$\begin{aligned} \sum_{\{u,v\} \subseteq V(J_m)} d(u,v)^2 &= m(1^2 + 1^2 + 1^2 + 2^2 + 2^2 + 2^2) \\ &+ \sum_{\substack{1 \le j < k \le m \\ k-j \le \lfloor \frac{m}{2} \rfloor}} \Big(3(k-j)^2 + 6(k-j+1)^2 + 7(k-j+2)^2\Big) \\ &+ \sum_{\substack{1 \le j < k \le m \\ k-j > \lfloor \frac{m}{2} \rfloor}} \Big(3(m-k+j)^2 + 6(m-k+j+1)^2 + 7(m-k+j+2)^2\Big). \end{aligned}$$

Next, we compute each of the terms

$$\sum(k-j)^2,\ \sum(k-j+1)^2,\ \sum(k-j+2)^2,\ \sum(m-k+j)^2,\ \sum(m-k+j+1)^2,\ \sum(m-k+j+2)^2$$

over their respectives ranges and obtain that

$$\sum_{\{u,v\} \subseteq V(J_m)} d(u,v)^2 = \begin{cases} \frac{m}{3}(2m^3 + 15m^2 + 55m - 6) & \text{if m even}, \\ \frac{m}{3}(2m^3 + 15m^2 + 49m - 21) & \text{if m odd.} \end{cases}.$$

Hence

$$HW(J_m) = \begin{cases} \frac{m}{3}(2m^3 + 21m^2 + 85m - 9) & \text{if m even}, \\ \frac{m}{3}(2m^3 + 21m^2 + 79m - 30) & \text{if m odd}. \end{cases}$$

□

5 Concluding remarks

For any two vertices $u, v \in V(G)$, $d(u/v)$ denotes the rational distance from u to v defined as

$$d(u/v) = \begin{cases} \sum_{u_i \in N[u]} \dfrac{d(u_i, v)}{deg(u) + 1} & \text{if} \quad u \neq v, \\ 0 & \text{if} \quad u = v, \end{cases}$$

where $N[u]$ is the closed neighborhood of u, and $deg(u)$ is the degree of u [1]. All the above invariants can also be determined using rational distance.

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