



## Zagreb Indices of the Thorn Jaco Graph Research Article

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**Abstract.** The first three Zagreb indices of a graph  $G$  denoted,  $M_1(G)$ ,  $M_2(G)$  and  $M_3(G)$ , are well known. In this paper we derive recursive formula for these indices for the family of thorn Jaco graphs. The concept of a *vertex invaded graph* is also introduced.

**Keywords.** Jaco graph; Thorn Jaco graph; Zagreb indices; Vertex invaded graph

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### 1. Introduction

For a general reference to notation and concepts of graph theory see [1]. For further reading we also refer to [2, 5]. The concept of linear Jaco graphs is well discussed in Kok et al. [6]. Finite linear Jaco graphs are derived from an infinite directed graph, called the  $f(x)$ -root digraph. The incidence function is a linear function  $f(x) = mx + c$ ,  $x \in \mathbb{N}$ ,  $m, c \in \mathbb{N}_0$ . The  $f(x)$ -root graph is denoted by  $J_\infty(f(x))$ . Much research has been done for the case  $f(x) = x$  hence, in respect of the linear Jaco graph  $J_n(x)$ ,  $n, x \in \mathbb{N}$ . For brevity, linear Jaco graphs are called *Jaco graphs*.

### 2. Finite Jaco Graphs

These directed graphs are derived from the infinite Jaco Graph called, the  $x$ -root digraph. The underlying graph will be denoted  $J_n^*(x)$  and if the context is clear, both the directed and undirected graphs are referred to as a *Jaco graph*. Similarly the difference between *arc* and *edge* and degree,  $d_{J_n(x)}(v)$  and  $d_{J_n^*(x)}(v)$  will be understood.

**Definition 2.1** ([6]). The infinite Jaco Graph  $J_\infty(x)$ ,  $x \in \mathbb{N}$  is defined by  $V(J_\infty(x)) = \{v_i : i \in \mathbb{N}\}$ ,  $A(J_\infty(x)) \subseteq \{(v_i, v_j) : i, j \in \mathbb{N}, i < j\}$  and  $(v_i, v_j) \in A(J_\infty(x))$  if and only if  $2i - d^-(v_i) \geq j$ .

**Definition 2.2** ([6]). The family of finite Jaco Graphs is defined by  $\{J_n(x) \subseteq J_\infty(x) : n, x \in \mathbb{N}\}$ . A member of the family is referred to as the Jaco Graph,  $J_n(x)$ .

**Definition 2.3** ([6]). The set of vertices attaining degree  $\Delta(J_n(x))$  is called the set of Jaconian vertices; the Jaconian vertices or the Jaconian set of the Jaco Graph  $J_n(x)$ , and denoted,  $\mathbb{J}(J_n(x))$  or,  $\mathbb{J}_n(x)$  for brevity.

**Definition 2.4** ([6]). The lowest numbered (subscripted) Jaconian vertex is called the prime Jaconian vertex of a Jaco Graph.

The  $x$ -root digraph has four fundamental properties which are:

- (i)  $V(J_\infty(x)) = \{v_i : i \in \mathbb{N}\}$ ,
- (ii) if  $v_j$  is the head of an arc then the tail is always a vertex  $v_i$ ,  $i < j$ ,
- (iii) if  $v_k$ , for smallest  $k \in \mathbb{N}$  is a tail vertex then all vertices  $v_\ell$ ,  $k < \ell < j$  are tails of arcs to  $v_j$ , and
- (iv) the degree of vertex  $v_k$  is  $d(v_k) = k$ .

The family of finite directed graphs are those limited to  $n \in \mathbb{N}$  vertices by lobbing off all vertices (and arcs to vertices)  $v_t$ ,  $t > n$ . Hence, trivially  $d(v_i) \leq i$  for  $i \in \mathbb{N}$ . Figure 1 depicts the  $J_{10}(x)$ .

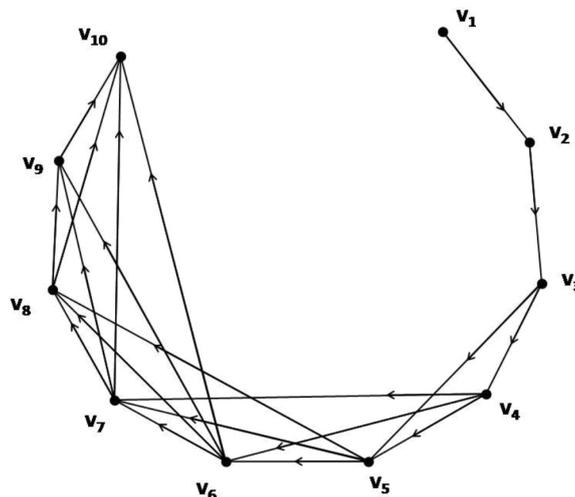


Figure 1. Jaco graph  $J_{10}(x)$ .

### 3. Zagreb Indices of Thorn Jaco Graphs

Recall that a thorn graph is defined by Gutman [4] is a graph  $G^*$  obtained from a graph  $G$  of order  $n$  by attaching  $s_i \geq 0$ ,  $i = 1, 2, \dots, n$ , pendant vertices to the  $i^{\text{th}}$  vertex of  $G$ . In this

paper  $s_i = d^-(v_i) \forall v_i \in V(J_n(x))$ . The motivation is that each vertex  $v_i, i \leq n$  is a source of some capacity transmission to the head vertices. To ensure that capacity transmission through to  $v_n$  is sustained, each vertex is allocated  $d^-(v_i)$  thorns as spare capacity sources.

For illustration the adapted table below follows from the Fisher algorithm [6] for  $J_n(x)$ ,  $n \leq 12$  and also depicts the degree sequence of  $J_n^*(x)$  denoted,  $\mathbb{D}(J_n^*(x))$ . Note that the entries of the degree sequence are in the consecutive order  $d(v_1), d(v_2), \dots, d(v_n)$ .

**Table 1**

$i \in \mathbb{N}$	$d^-(v_i)$	$d^+(v_i) = i - d^-(v_i)$	$\mathbb{D}(J_i^*(x))$
1	0	1	(0)
2	1	1	(1, 1)
3	1	2	(1, 2, 1)
4	1	3	(1, 2, 2, 1)
5	2	3	(1, 2, 3, 2, 2)
6	2	4	(1, 2, 3, 3, 3, 2)
7	3	4	(1, 2, 3, 4, 4, 3, 3)
8	3	5	(1, 2, 3, 4, 5, 4, 4, 3)
9	3	6	(1, 2, 3, 4, 5, 5, 5, 4, 3)
10	4	6	(1, 2, 3, 4, 5, 6, 6, 5, 4, 4)
11	4	7	(1, 2, 3, 4, 5, 6, 7, 6, 5, 5, 4)
12	4	8	(1, 2, 3, 4, 5, 6, 7, 7, 6, 6, 5, 4)

Although the formal algorithm to determine the degree sequence of  $J_i^*(x)$  is complex an easy *instrumental algorithm* can be derived directly from Table 1. Note that the last entry of the degree sequence of  $J_i^*(x)$  corresponds to  $d^-(v_i)$ . From Definition 2.1 it follows that the  $i^{\text{th}}$ -degree sequence increases consecutively to some maximum vertex degree. For illustration consider row 9 corresponding to  $\mathbb{D}(J_9^*(x))$ . Clearly the first five entries increase consecutively to a maximum value of 5. Constructing  $\mathbb{D}(J_{10}^*(x))$  means that the last four entries may each increase by 1 and a 10<sup>th</sup>-entry of 4 may be added. We further observe that the first entry say,  $k^{\text{th}}$  with maximum value  $j$ , hence  $d(v_k) = j$ , is the prime Jaconian vertex of the corresponding  $J_i^*(x)$ , ( $i^{\text{th}}$ -row) (see Definition 2.4). Also the subsequent entries equal to  $j$  correspond to the Jaconian set (see Definition 2.3). For example, for  $J_7^*(x)$  the Jaconian set is  $\{v_4, v_5\}$  and for  $J_{11}^*(x)$  it is  $\{v_7\}$ .

Following from Table 1 we summarise important observations as follow. If for  $n \in \mathbb{N}$  the degree sequence of  $J_n^*(x)$  is  $(1, 2, 3, \dots, p, q_1, q_2, \dots, q_t)$  then:

- (i)  $p + t = n$ ,
- (ii)  $v_p$  is the prime Jaconian vertex of  $J_n^*(x)$ ,
- (iii)  $p \geq q_1 \geq q_2$  and  $p > q_i, i = 3, 4, \dots, t$ ,
- (iv)  $d^-(v_n) = q_t$  hence,  $d^-(v_{n+1}) = t$ ,
- (v) the number of thorns allocated to  $v_j, j = 1, 2, 3, \dots, p, q_i, 1 \leq i \leq t$  remains equal in  $J_n^*(x)$  and  $J_{n+1}^*(x)$ ,
- (vi) The degree sequence of  $J_{n+1}^*(x)$  is  $(1, 2, 3, \dots, p, q_1 + 1, q_2 + 1, \dots, q_t + 1, t)$ ,
- (vii) In  $J_{n+1}^*(x)$  the vertex  $v_{n+1}$  is always allocated  $t$  thorns.

With regard to notation note the subtle difference between the underlying Jaco graph  $J_n^*(x)$  and the thorn Jaco graph  $J_n^*(x)$ .

### 3.1 Zagreb Indices

Recall that the first three Zagreb indices are defined to be:

$$M_1(G) = \sum_{v \in V(G)} d(v)^2 = \sum_{vu \in E(G)} (d(v) + d(u)),$$

$$M_2(G) = \sum_{vu \in E(G)} d(v)d(u),$$

$$M_3(G) = \sum_{vu \in E(G)} |d(v) - d(u)|.$$

**Proposition 3.1.** *The first Zagreb index of the thorn Jaco graph  $J_{n+1}^*(x)$  derived from  $M_1(J_n^*(x))$ , is:*

$$M_1(J_{n+1}^*(x)) = M_1(J_n^*(x)) + 2 \sum_{j=1}^t d_{J_n^*(x)}(v_{p+j}) + 2t(t+1).$$

*Proof.* The degree sequence of  $J_n(x)$ ,  $n \in \mathbb{N}$  can be expressed as  $(1, 2, 3, \dots, p, q_1, q_2, \dots, q_t)$ . Constructing a thorn graph  $J_n^*(x)$  with  $d^-(v_i)$  pendant vertices attached to each  $v_i \in V(J_n(x))$  results in:

$$M_1(J_n^*(x)) = \sum_{i=1}^p d_{J_n^*(x)}(v_i)^2 + \sum_{j=1}^t d_{J_n^*(x)}(v_{p+j})^2 + \sum_{k=1}^n d_{J_n^*(x)}^-(v_k).$$

In constructing  $J_{n+1}^*(x)$  the vertex  $v_{n+1}$  is added with  $t$  pendant vertices attached to  $v_{n+1}$  together with the edges,  $v_j v_{n+1}, 1 \leq j \leq t$ . Therefore:

$$\begin{aligned} M_1(J_{n+1}^*(x)) &= \sum_{i=1}^p d_{J_n^*(x)}(v_i)^2 + \sum_{j=1}^t (d_{J_n^*(x)}(v_{p+j}) + 1)^2 + \sum_{k=1}^n d_{J_n^*(x)}^-(v_k) + 4t^2 + t \\ &= M_1(J_n^*(x)) + 2 \sum_{j=1}^t d_{J_n^*(x)}(v_{p+j}) + 4t^2 + 2t. \end{aligned} \quad \square$$

### 3.2 Vertex Invaded Graph $G \uplus_\ell w$

Let  $G$  be a simple finite graph of order  $n$ . Let  $N_G(v)$  denote the open neighbourhood of  $v \in V(G)$ . Let the *vertex invaded* graph of  $G$  be the graph obtained by adding a new vertex  $w$  with edges to any number  $1 \leq \ell \leq n$  vertices of  $G$ . We also call a vertex invaded graph the 1-vertex invasion of a graph. Denote this vertex invaded graph by,  $G \uplus_\ell w$ . By adding  $\ell$  thorns to  $w$  we obtain a thorn graph  $G^* \uplus_\ell w$ . It is easy to see that path  $P_{n+1}$  is isomorphic to some  $P_n \uplus_1 v_{n+1}$  and the complete graph  $K_{n+1} = K_n \uplus_n v_{n+1}$ . Also the complete bipartite graph  $K_{m,n+1} = K_{m,n} \uplus_m v_{n+1}$ . But in general, for a connected graph  $G$  we have that after removal of a vertex  $v$  with  $d_G(v) = s$  that  $G$  is isomorphic to some  $(G - v) \uplus_s v$ . Clearly vertex invasion is not well-defined in that it does not derive a unique graph. In fact for a vertex labeled graph,  $G \uplus_\ell w \in \left\{ \frac{n!}{\ell!(n-\ell)!} \text{ possible graphs} \right\}$ . For an unlabeled graph the number of distinct vertex invaded graphs up to isomorphism can be noticeable less. Finding this number remains an open problem. The Pólya Enumeration Theorem, also known as the Redfield-Pólya Theorem might be key to solving this problem.

**Theorem 3.2.** For simple graph  $G$  of order  $n$  with second Zagreb index  $M_2(G)$  we have:

$$\begin{aligned}
 M_2(G^* \uplus_\ell w) &= M_2(G) + 4\ell^2 + 2\ell \sum_{i=1}^{\ell} d_G(v_i)_{v_i \in N(w)} \\
 &+ \sum_{\forall v_i \in N_{G^*}(w)} \left( \sum_{\forall u_j \in N_G(v_i), u_j \notin N(w)} d_G(u_j) \right) \\
 &+ \sum_{\lceil v_i, v_j \rceil \in \mathcal{T}(w)} (d_G(v_i) + d_G(v_j)) + |\mathcal{T}(w)|.
 \end{aligned}$$

*Proof.* Label the vertices  $v \in N_{G^*}(w)$  randomly as  $v_1, v_2, v_3, \dots, v_\ell$ , which is always possible. Clearly  $d_{G^*}(w) = 2\ell$ . Hence, from the definition of  $M_2(G^* \uplus_\ell w)$  the new sum-term  $\underbrace{2\ell \cdot 1 + 2\ell \cdot 1 + \dots + 2\ell \cdot 1}_{\ell\text{-terms}} = 2\ell^2$  is required in respect of the new thorns.

In respect of the edges  $wv_i, 1 \leq i \leq \ell$  the new sum-terms  $2\ell \sum_{i=1}^{\ell} (d_G(v_i) + 1) = 2\ell \sum_{i=1}^{\ell} d_G(v_i) + 2\ell^2$  are required.

Without loss of generality label the say  $m$  vertices in  $N_G(v_i)$  to be  $u_j, 1 \leq j \leq m_i$ .

*Case 1:* In respect of each  $v_i \in N_{G^*}(w)$  and each  $u_j \in N_G(v_i), u_j \notin N_{G^*}(w)$ , the new sum-terms come to the fore i.e.  $\sum_{j=1}^{m_i} (d_G(v_i) + 1)d_G(u_j)$ . On expansion of the summation to  $\sum_{j=1}^{m_i} d_G(v_i)d_G(u_j) +$

$\sum_{j=1}^{m_i} d_G(u_j)$  we note that the sum-term  $\sum_{j=1}^{m_i} d_G(v_i)d_G(u_j)$  has been accounted for in  $M_2(G)$ . Hence only the additional sum-term  $\sum_{\forall u_j \in N_G(v_i), u_j \notin N(w)} d_G(u_j)$  is required  $\forall v_i$ .

The aforesaid are the sum-terms  $\sum_{\forall v_i \in N_{G^*}(w)} \left( \sum_{\forall u_j \in N_G(v_i), u_j \notin N(w)} d_G(u_j) \right)$ . Therefore, the partial value of  $M_2(G^* \uplus_\ell w)$  is given by:

$$M_2(G) + 4\ell^2 + 2\ell \sum_{i=1}^{\ell} d_G(v_i)_{v_i \in N(w)} + \sum_{\forall v_i \in N_{G^*}(w)} \left( \sum_{\forall u_j \in N_G(v_i), u_j \notin N(w)} d_G(u_j) \right).$$

Case 2: In respect of each distinct pair of adjacent vertices  $\lceil v_i, v_j \rceil$ ,  $v_i, v_j \in N_{G^*}(w)$  the new sum terms  $d_G(v_i)d_G(v_j) + d_G(v_i) + d_G(v_j) + 1$  come to the fore. Since  $d_G(v_i)d_G(v_j)$  has been accounted for in  $M_2(G)$  only  $d_G(v_i) + d_G(v_j) + 1$  must be added for each such distinct pair of adjacent vertices. Denote the set of such distinct pairs of adjacent vertices,  $\mathcal{T}(w)$ .

Therefore

$$\begin{aligned} M_2(G^* \cup \ell w) &= M_2(G) + 4\ell^2 + 2\ell \sum_{i=1}^{\ell} d_G(v_i)_{v_i \in N(w)} \\ &+ \sum_{\forall v_i \in N_{G^*}(w)} \left( \sum_{\forall u_j \in N_G(v_i), u_j \notin N(w)} d_G(u_j) \right) \\ &+ \sum_{\lceil v_i, v_j \rceil \in \mathcal{T}(w)} (d_G(v_i) + d_G(v_j)) + |\mathcal{T}(w)|. \end{aligned}$$

That settles the result.  $\square$

We note that in terms of  $J_n^*(x)$  the thorn Jaco graph  $J_{n+1}^*(x)$  is indeed  $J_n^* \cup_{n-p} v_{n+1}$ . Furthermore, the vertices  $v_n, v_{n-1}, \dots, v_{p+1}$  adjacent to vertex  $v_{n+1}$  are well-defined. From this observation the next results follow.

**Proposition 3.3.** *The second Zagreb index of the thorn Jaco graph  $J_{n+1}^*(x)$  derived from  $M_2(J_n^*(x))$ , is:*

$$\begin{aligned} M_2(J_{n+1}^*(x)) &= M_2(J_n^*(x)) + 4(n-p)^2 + 2(n-p) \sum_{i=1}^{n-p} d_{J_n^*(x)}(v_{i+p}) \\ &+ \sum_{v_i, v_j \in V(\mathbb{H}(J_n^*(x)))} (d_{J_n^*(x)}(v_i) + d_{J_n^*(x)}(v_j)) + \frac{1}{2}(n-p)(n-p-1). \end{aligned}$$

*Proof.* Follows as a direct application of Theorem 3.2 with simplification.  $\square$

**Theorem 3.4.** *For simple graph  $G$  of order  $n$  with third Zagreb index  $M_3(G)$  we have:*

$$M_3(G^* \cup \ell w) = M_3(G) + \ell(2\ell - 1) + \sum_{i=1}^{\ell} |2\ell - (d_G(v_i) + 1)| + \sum_{\forall v_i, u_j \in E(G), v_i \in N_{G^*}(w), u_j \notin N_{G^*}(w)} 1. \quad 1.$$

*Proof.* The proof follows similar to that of Theorem 3.2.  $\square$

**Proposition 3.5.** *The third Zagreb index of the thorn Jaco graph  $J_{n+1}^*(x)$  derived from  $M_3(J_n^*(x))$ , is:*

$$\begin{aligned} M_3(J_{n+1}^*(x)) &= M_3(J_n^*(x)) + (n-p)(2(n-p) - 1) + \sum_{i=1}^{n-p} |2(n-p) - (d_{J_n^*(x)}(v_{i+p}) + 1)| \\ &+ \sum_{\forall v_i, u \in E(J_n^*(x)), v_i \in V(\mathbb{H}(J_n^*(x))), u \notin V(\mathbb{H}(J_n^*(x)))} 1. \end{aligned}$$

*Proof.* Follows as a direct application of Theorem 3.4.  $\square$

## 4. Conclusion

In the main the paper discusses Zagreb indices for a specific structured thorn Jaco graph. It is clear that despite the well-defineness of Jaco graphs, Zagreb indices are complex invariants to determine. Authors suggest that a wide scope for complexity analysis is available for worthy research.

The general result for graph invasion by a singular vertex proves to be complex. The concept can be generalised to model invasion by a finite number of vertices called  $n$ -vertex invasion. Clearly recursive algorithms will result from such generalisation. Application will be found in determining Zagreb indices for chemical derivatives of a given chemical compound modeled as graph  $G$ . For example regardless of the change in atom type, deriving butane,  $C_4H_{10}$  from methane,  $CH_4$  requires three, 3-vertex invasion iterations from a graph theoretic perspective.

### Competing Interests

The authors declare that they have no competing interests.

### Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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