Inverse Sum In-degree Index of Some Graphs and Their Squares

SHAHISTHA HANIF, K ARATHI BHAT* and SINCHANA NAGARAJ

***Abstract*—A topological index of a graph is a numeral value associated with a graph that fully uses it's topology and is invariant under graph isomorphism. There are certain important types of topological indices based on degree, distance, spectrum, and their mixed invariants. The inverse sum in-degree index (also known as ISI index) is one such degree-based topological index, defined with the intention that it may be useful in modeling molecular properties with higher accuracy than previously available descriptors. The ISI index of a graph G is defined as $ISI(G) = \sum_{v_i \sim v_j} \frac{d_G(v_i)d_G(v_j)}{d_G(v_i)+d_G(v_j)}$. In the similar line, the ISI-matrix $A_{ISI}(G) = (a_{ISI})_{ij}$ of G is a square matrix where $(a_{ISI})_{ij} = \frac{d_G(v_i)d_G(v_j)}{d_G(v_i)+d_G(v_j)}$ if $v_i \sim v_j$ and 0 otherwise. The article explores the ISI index of several classes of graphs and their squares. Other than the ISI index, some results on spectral properties and the determinant of the ISI matrix are derived. The article also gives bounds for the ISI index of certain type of bipartite graphs.**

***Index Terms*—Bi-star graph, Fan graph, Friendship graph, Spectral radius, Determinant.**

I. INTRODUCTION

A Topological index is generated by converting a molecular structure to a numeric value. In practical terms, the chemical compounds are taken as a graph where the atoms are vertices and the bonds connecting them are edges. These topological indices and their invariants are utilized in quantitative structure–property relationships (QSPR), structure-activity relationships (QSAR), and structural design in chemistry, nanotechnology, and pharmacology.

The first topological index is the Wiener index, which was introduced by H Wiener in 1947. The Wiener index was used to determine the physical properties of paraffins [1]. The journey of degree-based indices began through Zagreb indices to provide a quantitative assessment of molecular branching, which then led to a significant variety of useful indices. The first Zagreb index is the most studied index, which was defined by Gutman and Trinajstic [2]. Hundreds of topological indices are currently being researched and developed in the literature of mathematical chemistry due to their extensive applications. Though a lot many topological indices have been defined based on degree, distance, eccentricity, and so on, yet not all of them have been found to be significant. On the other hand, the ISI index is found to have a special impetus as a predictor of the total surface area of octane isomers. Out of the 148 discrete Adriatic indices studied in 2010, the ISI index finds its place in the list of twenty indices selected as significant predictors.

For a graph $G = (V, G)$ with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, the degree and neighborhood of v_i are denoted by $d_G(v_i)$ and $N_G(v_i)$, respectively. We write $v_i \sim v_j$ if v_i and v_j are adjacent, and $v_i \nsim v_j$ if not. The adjacency matrix (also known as classical adjacency matrix) $A(G) = (a_{ij})$ is a square matrix of order n where $a_{ij} = 1$ if $v_i \sim v_j$ and 0 otherwise. The eigenvalues of $A(G)$ associated with their multiplicities compose the spectrum of G.

The inverse sum in-degree index of a graph G, is defined as

$$ISI(G) = \sum_{v_i \sim v_j} \frac{d_G(v_i)d_G(v_j)}{d_G(v_i)+d_G(v_j)} \tag{1}$$

Several extended adjacency matrix corresponding to a degree based topological index are studied in literature [10]–[12].

The ISI-matrix $A_{ISI}(G) = (a_{ISI})_{ij}$ of a graph G of order n is a square matrix where $(a_{ISI})_{ij} = \frac{d_G(v_i)d_G(v_j)}{d_G(v_i)+d_G(v_j)}$ if $v_i \sim v_j$ and 0 otherwise. The eigenvalues of ISI matrix $A_{ISI}(G)$ associated with their multiplicities are called the ISI-spectrum of G. Significant studies on ISI index of various types of graphs and various types of graph operations have been carried out in the literature (refer [3], [4], [5], [6], [7], [8], [9]). The ISI index of some of the standard graph classes like path graphs, complete graphs, etc. are listed out here, which will be used in the latter part of the article. For a path graph P_n, a complete graph K_n, a cycle graph C_n, a wheel graph $W_{1,n-1}$ on n vertices, and a complete bipartite graph $K_{m,n}$ on $m+n$ vertices, the ISI index are

- $ISI(P_n) = \dfrac{3n-5}{3}$
- $ISI(C_n) = n$
- $ISI(K_n) = \dfrac{n(n-1)^2}{4}$
- $ISI(W_{1,n-1}) = \dfrac{9n(n-1)}{2(n+2)}$
- $ISI(K_{m,n}) = \dfrac{m^2n^2}{m+n}$.

II. SQUARE OF STANDARD CLASSES OF GRAPHS

The square of a graph G, denoted by G^2, has the same set of vertices as G, and any two vertices $v_i \sim v_j$ in G^2 if and only if they are joined in G by a path of length one or two. Graph powers are useful in distributed computing and designing algorithms for certain combinatorial optimization problems [13]. The rigidity of squares of graphs in three-space has important applications to the study of flexibility in molecules [14].

Since $V(G) = V(G^2)$ and G^2 has all the edges of G, on squaring a graph G, additional edges are added without

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changing the labels of the vertices of G. This convention is just for the simplicity in understanding the proofs, as the ISI matrix is indexed by vertices of graphs. Note that, if G is a graph having diameter 2, then G^2 is a complete graph.

The following lemma uses the relation between the classical adjacency matrix and ISI matrix of a graph when the graph G is regular and derives the expression for ISI index, determinant and spectral radius of $A_{ISI}(G)$.

Lemma 2.1: Let G be an $r-$regular graph on n vertices. Let $A(G)$ and $A_{ISI}(G)$ be the classical adjacency matrix and the ISI matrix, respectively. Then

$$ISI(G) = \frac{nr^2}{4}$$
$$det(A_{ISI}(G)) = \left(\frac{r}{2}\right)^n det(A(G))$$
$$\tau_{n-1}(A_{ISI}(G)) = \frac{r^2}{2}$$

where $det(A), det(A_{ISI}(G))$ are the determinant of the matrices $A(G), A_{ISI}(G)$, respectively and $\tau_{n-1}(A_{ISI}(G))$ is the spectral radius of $A_{ISI}(G)$.

Proof: Since G is $r-$regular, the only non-zero entries of $A_{ISI}(G)$ are $\frac{r}{2}$. Further, the number of edges in G is $\frac{nr}{2}$. Thus $A_{ISI}(G)$ has $\frac{nr}{2}$ nonzero entries, each of which is $\frac{r}{2}$. Thus $ISI(G) = \frac{nr^2}{4}$. Further, $A_{ISI}(G) = \frac{r}{2}A(G)$ and $det(A_{ISI}(G)) = \left(\frac{r}{2}\right)^n det(A(G))$. Since G is $r-$ regular, it is true that r is the spectral radius of $A(G)$, which implies $\frac{r^2}{2}$ is the spectral radius of $A_{ISI}(G)$. ■

Theorem 2.2: Let P_n be a path graph and $G = P_n^2$ where $n \geq 6$. Then

$$ISI(G) = \frac{420n - 1058}{105}.$$

Proof: We know that $|V(G)| = |V(P_n)| = n$ and $|E(G)| = 2n - 3$. Let the vertices of P_n be labelled as $v_1, v_2, \ldots, v_n$ (v_1 and v_n being the pendant vertices), then the degrees of vertices $v_1, v_2, \ldots, v_n$ in G are $2, 3, \underbrace{4, 4, \ldots, 4}_{(n-4\ times)}, 3, 2$, respectively. The ISI matrix $A_{ISI}(G)$, whose rows and columns are indexed by the vertices $v_1, v_2, \ldots, v_n$ has only $2(2n-3)$ non-zero entries. The non-zero entries $(a_{ISI})_{ij}$ of $A_{ISI}(G)$ are given by $\frac{6}{5}\left[(a_{ISI})_{12}, (a_{ISI})_{(n-1)n}\right]$, $\frac{8}{6}\left[(a_{ISI})_{13}, (a_{ISI})_{(n-2)n}\right]$, $\frac{12}{7}\left[(a_{ISI})_{23}, (a_{ISI})_{24}, (a_{ISI})_{(n-2)(n-1)}, (a_{ISI})_{(n-3)(n-1)}\right]$ and the remaining $(2n-11)$ entries given by $\frac{16}{8}$. Since the matrix $A_{ISI}(G)$ symmetric, we have

$$\begin{aligned} ISI(G) &= 2 \times \frac{6}{5} + 2 \times \frac{8}{6} + 4 \times \frac{12}{7} + (2n-11) \times \frac{16}{8} \\ &= \frac{420n - 1058}{105}. \end{aligned}$$

■

For all the path graphs on $n < 6$ vertices, that is, when $n = 2, 3, 4, 5$, one can easily evaluate the ISI index as $0.5, 3, \frac{63}{10}$ and $\frac{2099}{210}$, respectively.

Theorem 2.3: Let C_n be a cycle graph and $G = C_n^2$ where $n \geq 5$. Then

$$ISI(G) = 4n$$
$$det(A_{ISI}(G)) = \begin{cases} 2^{n+2} & n \cong 1 \mod 6 \ or\ n \cong 5 \mod 6 \\ 2^{n+4} & n \cong 3 \mod 6 \\ 0 & else \end{cases}$$
$$\tau_{n-1}(A_{ISI}(G)) = 8.$$

Proof: The graph G is a 4-regular graph and hence by Lemma 2.1, $ISI(G) = 4n$ and $\tau_{n-1}(A_{ISI}(G)) = 8$. Further, the determinant also follows from Lemma 2.1 and the fact that the adjacency matrix $A(G)$ of G, is a circulant matrix given by $A = circulant(0, 1, 1, 0, 0, \ldots, 0, 0, 1, 1)$ whose determinant is

$$det(A(G)) = \begin{cases} 4 & n \cong 1 \mod 6 \ or\ n \cong 5 \mod 6 \\ 16 & n \cong 3 \mod 6 \\ 0 & else. \end{cases}$$

■

When $n = 3, 4$, the graphs G_n^2 are complete graphs K_3, K_4, respectively.

Corollary 2.4: Let C_n be a cycle graph and $G = C_n^2$ for $n \geq 6$. Then spectrum of $A_{ISI}(G)$ is given by

$$spec\left[A_{ISI}(G)\right] = \{\tau_{n-1}, \tau_{n-2}, \ldots, \tau_2, \tau_1, \tau_0\},$$

where $\tau_j = \omega^j + \omega^{2j} + \omega^{(n-2)j} + \omega^{(n-1)j}$, where $w = e^{\frac{2\pi i}{n}}$ for $0 \leq j \leq (n-1)$.

Proof: The ISI matrix $A_{ISI}(G)$ is a circulant matrix given by

$$A_{ISI}(G) = circulant(0, 2, 2, 0, 0, \ldots, 0, 0, 2, 2),$$

the spectrum of which can derived form the following property of circulant matrices: "If A is a circulant matrix $A = circulant(c_0, c_1, \ldots, c_{n-1}, c_n)$, then the eigenvalues λ_j $(0 \leq j \leq n-1)$ are given by $\lambda_j = c_0 + c_1\omega^j + c_2\omega^{2j} + \cdots + c_{n-1}^{(n-1)j}$ where $\omega = e^{\frac{2\pi i}{n}}$ ". ■

Theorem 2.5: Let $K_{m,n}$ and $W_{1,n}$ be the complete bipartite graph and wheel graph respectively. If $G = K_{m,n}^2$ and $H = W_{1,n}^2$, then

$$ISI(G) = \frac{(m+n-1)^2(m+n)}{4}$$
$$ISI(H) = \frac{n^2(n+1)}{4}.$$

Proof: Since $K_{m,n}$ and $W_{1,n}$ have diameter 2, the graphs G, H are given by $G = K_{m+n}$ and $H = K_{n+1}$, the complete graphs on $(m+n)$ and $(n+1)$, respectively. The statement follows as the ISI index of complete graph K_n on n vertices is $\frac{n(n-1)^2}{4}$. ■

Remark 2.1: If $G = K_{1,n}^2$, where $K_{1,n}$ is a star graph, then,

$$ISI(G) = \frac{n^2}{n+1}.$$

Theorem 2.6: Let $G = K_{m,n}^2$ and $H = W_{1,n}^2$, where $K_{m,n}$ and $W_{1,n}$ are the complete bipartite graph and wheel graph respectively. Then

$$det(A_{ISI}(G)) = \frac{(-1)^{m+n-1}(m+n-1)^{m+n+1}}{2^{m+n}}$$
$$det(A_{ISI}(H)) = \frac{(-1)^n n^{n+2}}{2^{n+1}}$$

and

$$\tau_{n-1}(A_{ISI}(G)) = \frac{(m+n+1)^2}{2}$$
$$\tau_{n-1}(A_{ISI}(H)) = \frac{n^2}{2},$$

where τ_{n-1} is the spectral radius.

Proof: Since G is a $(m+n-1)$ regular graph, by Lemma 2.1,
$det(A_{ISI}(G)) = det(A_{ISI}(K_{m+n})) = \frac{(m+n-1)^{m+n}}{2^{m+n}} det(A(G))$,
where $A(G)$ is the adjacency matrix of G. As the determinant of the adjacency matrix of a complete graph K_{m+n} is $det(A(G)) = det(K_{m+n}) = (-1)^n(n-1)$, the proof follows. Similarly, $det(A_{ISI}(G)) = det(A_{ISI}(K_{n+1}))$ can be derived.
The spectral radius for both the graphs G and H follow directly from Lemma 2.1. ■

III. Some new classes and their squares

In this section, the ISI index of some unexplored classes of graphs like fan graphs, friendship graphs and bi-star graphs and their squares are derived. A fan graph $F_{1,n}$ is obtained by joining all vertices of path P_n, to a further vertex (called the centre or the central vertex) by edges (refer Figure 1).

Theorem 3.1: Let $F_{1,n}$ be a fan graph and $G = F_{1,n}^2$. Then

$$ISI(F_{1,n}) = \frac{45n^3 + 94n^2 - 15n - 126}{10(n^2 + 5n + 6)}$$
$$ISI(G) = \frac{n^2(n+1)}{4}.$$

Proof: The fan graph $F_{1,n}$ has $(n+1)$ vertices, out of which one vertex, say v_1 is of degree n and two vertices, say v_2, v_{n+1} are of degree 2 and remaining vertices $v_3, v_4, \ldots, v_n$ of degree 3. The ISI matrix $A_{ISI}(F_{1,n})$ whose rows and columns are indexed by $v_1, v_2, \ldots, v_n, v_{n+1}$ has $(4n-2)$ no zero entries as shown below.

$$\begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ \vdots \\ v_n \\ v_{n+1} \end{array}
\begin{array}{c}
\begin{array}{ccccccc} v_1 & v_2 & v_3 & v_4 & \ldots & v_n & v_{n+1} \end{array} \\
\begin{pmatrix}
0 & \frac{2n}{2+n} & \frac{3n}{3+n} & \frac{3n}{3+n} & \ldots & \frac{3n}{3+n} & \frac{3n}{3+n} \\
\frac{2n}{2+n} & 0 & \frac{6}{5} & 0 & \ldots & 0 & 0 \\
\frac{3n}{3+n} & \frac{6}{5} & 0 & \frac{9}{6} & \ldots & 0 & 0 \\
\frac{3n}{3+n} & 0 & \frac{9}{6} & 0 & \ldots & 0 & 0 \\
\vdots & \vdots & & & & & \\
\frac{3n}{3+n} & 0 & 0 & 0 & \ldots & 0 & \frac{6}{5} \\
\frac{2n}{2+n} & 0 & 0 & 0 & \ldots & \frac{6}{5} & 0
\end{pmatrix}
\end{array}$$

The nonzero entries of $A_{ISI}(G)$ are given by: $\frac{2n}{2+n}\left[(a_{ISI})_{12} \text{ and } (a_{ISI})_{1(n+1)}\right]$, $\frac{3n}{3+n}\left[(a_{ISI})_{1k}; 3 \le k \le n\right]$, $\frac{6}{5}\left[(a_{ISI})_{23} \text{ and } (a_{ISI})_{n(n+1)}\right]$ and $\frac{9}{6}\left[(a_{ISI})_{k(k+1)}; 3 \le k \le n-1\right]$. Thus

$$\begin{aligned} ISI(F_{1,n}) &= 2 \times \frac{2n}{2+n} + (n-2) \times \frac{3n}{3+n} + 2 \times \frac{6}{5} \\ &\quad + (n-3) \times \frac{9}{6} \\ &= \frac{45n^3 + 94n^2 - 15n - 126}{10(n^2 + 5n + 6)}. \end{aligned}$$

Further, since diameter of $F_{1,n}$ is 2, the graph $G = F_{1,n}^2$ is a complete graph on $(n+1)$ vertices, the ISI index is given by

$$ISI(G) = \frac{n^2(n+1)}{4}.$$

■

A friendship graph F_n can be constructed by joining n copies of the cycle graph C_3 with a common vertex, which is also called the central vertex. Hence, F_n has $(2n+1)$ vertices and $3n$ edges. In graph F_n, every two distinct vertices have exactly one common adjacent vertex (refer Figure 1).

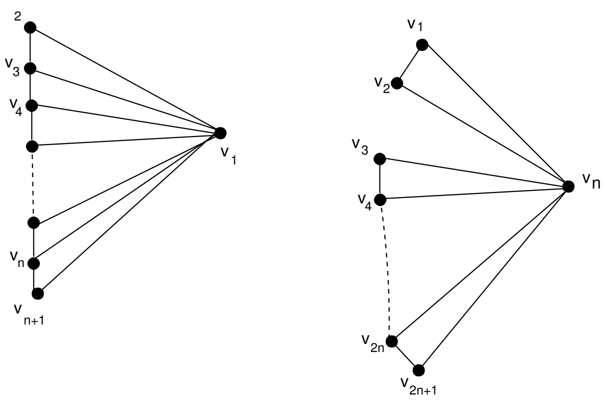

Fig. 1. Fan graph F_n(left) and friendship graph $F_{1,n}$(right)

Theorem 3.2: Let F_n be a friendship graph and $G = F_n^2$. Then

$$ISI(F_n) = \frac{5n^2 + n}{n+1}$$
$$ISI(G) = n^2(2n+1).$$

Proof: Let v_1 be the central vertex of F_n, which is of degree $2n$. The remaining vertices, say $v_2, v_3, \ldots, v_{2n+1}$ have degree 2. All the entries of the matrix $A_{ISI}(F_n)$ are zero except $(a_{ISI})_{1k}$ for $2 \le k \le (2n+1)$ $\left[(a_{ISI})_{1k} = \frac{4n}{2+2n}\right]$ and $(a_{ISI})_{k(k+1)}$ for all even integers $2 \le k \le 2n$ $[(a_{ISI})_{1k} = 1]$. Thus

$$\begin{aligned} ISI(F_n) &= 2n \times \frac{4n}{2+2n} + n \\ &= \frac{5n^2 + n}{n+1}. \end{aligned}$$

Since $G = K_{2n+1}$, $ISI(G)$ follows. ■

Theorem 3.3: Let F_n be a friendship graph and $A_{ISI}(F_n)$ be the ISI matrix of F_n. Then $-1, +1$ are the eigenvalues of $A_{ISI}(F_n)$ with respective multiplicities n and $(n-1)$.

Proof: The matrix $A_{ISI}(F_n)$ is a $(2n+1) \times (2n+1)$

matrix, given by

$$\begin{array}{cc} & \begin{matrix} C_1 & C_2 & C_3 & C_4 & \dots & C_{2n} & C_{2n+1} \end{matrix} \\ \begin{matrix} R_1 \\ R_2 \\ R_3 \\ R_4 \\ \vdots \\ R_{2n} \\ R_{2n+1} \end{matrix} & \begin{pmatrix} 0 & \frac{2n}{n+1} & \frac{2n}{n+1} & \frac{2n}{n+1} & \dots & \frac{2n}{n+1} & \frac{2n}{n+1} \\ \frac{2n}{n+1} & 0 & 1 & 0 & \dots & 0 & 0 \\ \frac{2n}{n+1} & 0 & 0 & 0 & \dots & 0 & 0 \\ \frac{2n}{n+1} & 0 & 0 & 1 & \dots & 0 & 0 \\ \vdots & & & & & & \\ \frac{2n}{n+1} & 0 & 0 & 0 & \dots & 0 & 1 \\ \frac{2n}{n+1} & 0 & 0 & 0 & \dots & 1 & 0 \end{pmatrix} \end{array}$$

Let the rows and columns of $A_{ISI}(F_n)$ (indexed by the vertices $v_1, v_2, \dots, v_{2n+1}$) be named as $R_1, R_2, R_3, \dots, R_{2n+1}$ and $C_1, C_2, C_3, \dots, C_{2n+1}$ as shown. Now, consider $(A_{ISI}(F_n) - \tau I)$, where τ is eigenvalue and follows the given sequence of row and column operations.

Step 1: $R_j = R_j - R_{j-1}$ for $j = 3, 5, 7, 9, \dots, (2n+1)$. We get $det(A_{ISI}(F_n) - \tau I) = (\tau + 1)^n det(B)$, where B is a $(2n+1) \times (2n+1)$ matrix given by

$$B = \begin{pmatrix} -\tau & \frac{2n}{n+1} & \frac{2n}{n+1} & \frac{2n}{n+1} & \cdots & \frac{2n}{n+1} & \frac{2n}{n+1} \\ \frac{2n}{n+1} & -\tau & 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & -1 & 0 & \dots & 0 & 0 \\ \frac{2n}{n+1} & 0 & 0 & -\tau & \dots & 0 & 0 \\ 0 & 0 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & & & & & \\ \frac{2n}{n+1} & 0 & 0 & 0 & \dots & -\tau & 1 \\ 0 & 0 & 0 & 0 & \dots & 1 & -1 \end{pmatrix}$$

Step 2: $C_k = C_k + C_{k+1}$ for $k = 2, 4, 6, \dots, 2n$. Then $det(A_{ISI}(F_n) - \tau I) = (\tau + 1)^n C$, where C is

$$\begin{pmatrix} -\tau & \frac{4n}{n+1} & \frac{2n}{n+1} & \frac{4n}{n+1} & \cdots & \frac{4n}{n+1} & \frac{2n}{n+1} \\ \frac{2n}{n+1} & 1-\tau & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & -1 & 0 & \dots & 0 & 0 \\ \frac{2n}{n+1} & 0 & 0 & 1-\tau & \dots & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & & & & & \\ \frac{2n}{n+1} & 0 & 0 & 0 & \dots & 1-\tau & 1 \\ 0 & 0 & 0 & 0 & \dots & 0 & -1 \end{pmatrix}$$

The i^{th} row of C has only one non-zero entry -1 at i^{th} position for every odd integer $3 \leq i \leq (2n+1)$.

Step 3: Expand the determinant of C along the rows $R_3, R_5, R_7 \dots R_{2n+1}$ sequentially. Then $det(A_{ISI}(F_n)) = (-1)^n (\tau + 1)^n det(D)$, where D is an $(n+1) \times (n+1)$ matrix given by

$$\begin{pmatrix} -\tau & \frac{4n}{n+1} & \frac{4n}{n+1} & \frac{4n}{n+1} & \cdots & \frac{4n}{n+1} & \frac{4n}{n+1} \\ \frac{2n}{n+1} & 1-\tau & 0 & 0 & \dots & 0 & 0 \\ \frac{2n}{n+1} & 0 & 1-\tau & 0 & \dots & 0 & 0 \\ \frac{2n}{n+1} & 0 & 0 & 1-\tau & \dots & 0 & 0 \\ \frac{2n}{n+1} & 0 & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & & & & & \\ \frac{2n}{n+1} & 0 & 0 & 0 & \dots & 1-\tau & 0 \\ \frac{2n}{n+1} & 0 & 0 & 0 & \dots & 0 & 1-\tau \end{pmatrix}$$

Let the rows and columns of D be indexed by $R_1^{'}, R_2^{'} \dots, R_{n+1}^{'}$ and $C_1^{'}, C_2^{'} \dots, C_{n+1}^{'}$.

Step 4: $R_i^{'} = R_i^{'} - R_{i-1}^{'}$ for $i = 3, 4, 5, 6, \dots, (n+1)$. Then $det(A_{ISI}(F_n)) = (-1)^n (\tau + 1)^n (\tau - 1)^{n-1} det(E)$, where E is

$$\begin{pmatrix} -\tau & \frac{4n}{n+1} & \frac{4n}{n+1} & \frac{4n}{n+1} & \cdots & \frac{4n}{n+1} & \frac{4n}{n+1} \\ \frac{2n}{n+1} & 1-\tau & 0 & 0 & \dots & 0 & 0 \\ 0 & 1 & -1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & -1 & \dots & 0 & 0 \\ 0 & 0 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & & & & & \\ 0 & 0 & 0 & 0 & \dots & 1 & -1 \\ \frac{2n}{n+1} & 0 & 0 & 0 & \dots & 0 & 1-\tau \end{pmatrix}$$

Since the characteristic polynomial of $A_{ISI}(F_n)$ has the factors $(\tau + 1)^n$ and $(\tau - 1)^{n-1}$, the theorem follows. ■

A bi-star graph $B(p, q)$ is a bipartite graph obtained by joining the central vertices of two star graphs $K_{1,p-1}$ and $K_{1,q-1}$ by an edge (refer Figure 2). The bi-star graph $B(p, q)$ has bipartition $V(B(p, q)) = V_1 \cup V_2$ with cardinalities p ($|V_1| = p$) and q ($|V_2| = q$), each containing exactly one central vertex of the star graphs. Clearly, each of the partite sets have exactly one vertex (the central vertices of star graphs) which is adjacent with all vertices of the other partite set. These vertices are often known as dominating vertices.

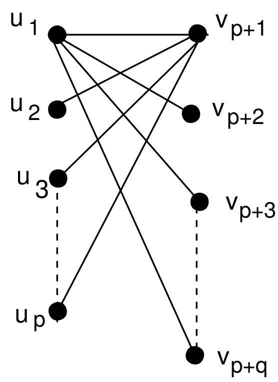

Fig. 2. Bi-star graph $B(p, q)$ with dominating vertices u_1 and v_{p+1}

Theorem 3.4: Let $B(p, q)$ be a bi-star graph and $G =$

$B(p,q)^2$. Then

$$
\begin{aligned}
ISI(B(p,q)) &= \frac{pq}{p+q} + \frac{p(p-1)}{p+1} + \frac{q(q-1)}{q+1},\\
ISI(G) &= \frac{n-1}{2} + \frac{q(q-1)\left[q^2+(n-3)q+2(n-1)\right]}{4(n+q-1)}\\
&\quad + \frac{p(p-1)\left[p^2+(n-3)p+2(n-1)\right]}{4(n+p-1)}.
\end{aligned}
$$

Proof: Let the graph $B(p,q)$ has the bipartition $V(B(p,q)) = V_1 \cup V_2$, where $V_1 = \{u_1, u_2, \ldots, u_p\}$ and $V_2 = \{v_{p+1}, v_{p+2}, \ldots, v_{p+q}\}$. Let u_1, v_{p+1} be the dominating vertices of V_1, V_2, respectively. Further, the degrees of u_i, v_j are 1 for all $2 \le i \le p$ and $(p+2) \le j \le (p+q)$. The ISI matrix $A_{ISI}(B(p,q))$ has only $2(p+q-1)$ nonzero entries, given by $\frac{pq}{p+q}$ for $(a_{ISI})_{1(p+1)}$, $\frac{q}{q+1}$ for $(a_{ISI})_{1j}$ for $(p+2) \le j \le (p+q)$ and $\frac{p}{p+1}$ for $(a_{ISI})_{i(p+1)}$ $2 \le i \le p$. Thus

$$
\begin{aligned}
ISI(B(p,q)) &= \frac{pq}{p+q} + (q-1)\times\frac{q}{q+1} + (p-1)\times\frac{p}{p+1}\\
&= \frac{pq}{p+q} + \frac{p(p-1)}{p+1} + \frac{q(q-1)}{q+1}
\end{aligned}
$$

On retaining the same labels in $G = B(p,q)^2$, the degrees of the vertices will be altered as follows: $d_G(u_1) = d_G(v_{p+1}) = p+q-1$, $d_G(u_i) = p$ for $1 \le i \le p$, $d_G(v_j) = q$ for $(p+2) \le j \le (p+q)$. Both V_1 and V_2 induce cliques of size p, q respectively and no other new edges connecting the vertices of V_1 with V_2 are added. Thus $A_{ISI}(G)$ has only $2\left(\frac{p(p-1)}{2} + \frac{q(q-1)}{2} + (p+q-1)\right)$ non-zero entries given by
$(a_{ISI})_{1(p+1)} = \frac{(p+q-1)^2}{2p+2q-2}$,
$(a_{ISI})_{1j} = \frac{q(p+q-1)}{p+2q-1}$ for $(p+2) \le j \le (p+q)$,
$(a_{ISI})_{i(p+1)} = \frac{p(p+q-1)}{2p+q-1}$ for $2 \le i \le p$,
$(a_{ISI})_{ik} = \frac{p}{2}$ for $2 \le i \le p$, $2 \le k \le p$ with $i \ne k$ and $(a_{ISI})_{jk} = \frac{q}{2}$ for $2 \le j \le q$ and $2 \le k \le q$ with $j \ne k$. Thus

$$
\begin{aligned}
ISI(G) &= \frac{(p+q-1)^2}{2p+2q-2} + (q-1)\times\frac{q(p+q-1)}{p+2q-1} +\\
&\quad (p-1)\times\frac{p(p+q-1)}{2p+q-1} + \binom{p-1}{2}\frac{p}{2} + \binom{q-1}{2}\frac{q}{2}\\
&= \frac{n-1}{2} + \frac{q(q-1)\left[q^2+(n-3)q+2(n-1)\right]}{4(n+q-1)} +\\
&\quad \frac{p(p-1)\left[p^2+(n-3)p+2(n-1)\right]}{4(n+p-1)}
\end{aligned}
$$

■

Theorem 3.5: Let $B(p,q)$ be a bi-star graph with ISI matrix $A_{ISI}(B(p,q))$. Then $A_{ISI}(B(p,q))$ is singular. That is, 0 is an eigenvalue of $A_{ISI}(B(p,q))$ with multiplicity $(p+q-4)$

Proof: The ISI matrix of $B(p,q)$ is a matrix of order $(p+q-1)$, given by $A_{ISI}(B_{p,q}) =$

$$
\begin{array}{cc}
 & \begin{array}{cccccccc} C_1 & C_2 & \dots & C_p & C_{p+1} & C_{p+2} & \dots & C_{p+q} \end{array}\\
\begin{array}{c} R_1\\ R_2\\ R_3\\ \vdots\\ R_p\\ R_{p+1}\\ R_{p+2}\\ R_{p+3}\\ \vdots\\ R_{p+q} \end{array} &
\begin{pmatrix}
0 & 0 & \dots & 0 & \frac{pq}{p+q} & \frac{q}{q+1} & \dots & \frac{q}{q+1}\\
0 & 0 & \dots & 0 & \frac{q}{q+1} & 0 & \dots & 0\\
0 & 0 & \dots & 0 & \frac{q}{q+1} & 0 & \dots & 0\\
\vdots & & & & & & & \\
0 & 0 & \dots & 0 & \frac{q}{q+1} & 0 & \dots & 0\\
\frac{pq}{p+q} & \frac{p}{p+1} & \dots & \frac{p}{p+1} & 0 & 0 & \dots & 0\\
\frac{p}{p+1} & 0 & \dots & 0 & 0 & 0 & \dots & 0\\
\frac{p}{p+1} & 0 & \dots & 0 & 0 & 0 & \dots & 0\\
\vdots & & & & & & & \\
\frac{p}{p+1} & 0 & \dots & 0 & 0 & 0 & \dots & 0
\end{pmatrix}
\end{array}
$$

Let the rows and columns of $A_{ISI}(B_{p,q})$ (indexed by vertices $u_1, u_2, \ldots, u_p, v_{p+1}, v_{p+2}, \ldots, v_{p+q}$) be named as $R_1, R_2, \ldots, R_p, R_{p+1}, R_{p+3} \ldots, R_{p+q}$ and $C_1, C_2, \ldots, C_p, C_{p+1}, C_{p+2}, \ldots, C_{P+q}$ as shown. Now, consider $(A_{ISI}(B(p,q) - \tau I)$ and do the row operations $R_i = R_i - R_{i-1}$ for $3 \le i \le p$ and $(p+3) \le i \le (p+q)$. Subsequently, we get

$$det\left[A_{ISI}(B(p,q) - \tau I\right] = \tau^{p+q-4} det(B),$$

where B is

$$
\begin{array}{cc}
 & \begin{array}{cccccccc} C_1 & C_2 & \dots & C_{p+1} & C_{p+2} & \dots & C_{p+q-1} & C_{p+q} \end{array}\\
\begin{array}{c} R_1\\ R_2\\ R_3\\ \vdots\\ R_p\\ R_{p+1}\\ R_{p+2}\\ R_{p+3}\\ \vdots\\ R_{p+q} \end{array} &
\begin{pmatrix}
-\tau & 0 & \dots & \frac{pq}{p+q} & \frac{q}{q+1} & \dots & \frac{q}{q+1} & \frac{q}{q+1}\\
0 & -\tau & \dots & \frac{q}{q+1} & 0 & \dots & 0 & 0\\
0 & 1 & \dots & \frac{q}{q+1} & 0 & \dots & 0 & 0\\
\vdots & & & & & & & \\
0 & 0 & \dots & \frac{q}{q+1} & 0 & \dots & 0 & 0\\
\frac{pq}{p+q} & \dots & \frac{p}{p+1} & -\tau & 0 & \dots & 0 & 0\\
\frac{p}{p+1} & 0 & \dots & 0 & -\tau & \dots & 0 & 0\\
0 & 0 & \dots & 1 & -1 & \dots & 0 & 0\\
\vdots & & & & & & & \\
0 & 0 & \dots & 0 & 0 & \dots & 1 & -1
\end{pmatrix}
\end{array}
$$

■

The helm graph H_n is the graph obtained from a wheel graph $W_{1,n}$ by adjoining a pendant edge at each vertex of the cycle.A helm graph H_n has $(2n+1)$ vertices among which 1 vertex of degree n, n vertices of degree 4 and n pedant vertices. Helm graph H_n is shown in Figure 3.

Theorem 3.6: If H_n is a helm graph, then

$$ISI(H_n) = \frac{n(34n+56)}{5(4+n)}.$$

Proof: Let v_1 be the central vertex of degree n, $v_2, v_3 \ldots, v_{n+1}$ be the internal vertices of degree 4 and $u_{n+2}, u_{n+3}, \ldots, u_{2n+1}$ be the pendant vertices. Since there are vertices with only three distinct degrees, the ISI matrix $A_{ISI}(H_n)$ has only $6n$ nonzero entries, given by $\frac{4n}{4+n}$ for $(a_{ISI})_{1i}$ for $2 \le i \le n+1$, 2 for $(a_{ISI})_{j(j+1)}$ for $2 \le j \le$

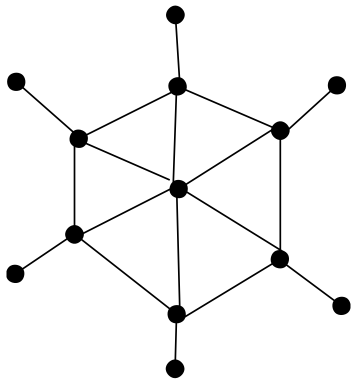

Fig. 3. Helm graph H_6

n, 2 for $(a_{ISI})_{2(n+1)}$ and $\frac{4}{5}$ for $(a_{ISI})_{j(n+j)}$ $2 \leq i \leq p$. Thus

$$\begin{aligned} ISI(H_n) &= n \times \frac{4n}{4+n} + n \times 2 + n \times \frac{4}{5} \\ &= \frac{n(34n+56)}{5(4+n)}. \end{aligned}$$

■

The square of helm graphs are considered at the end of this section. The next theorem gives the bounds for ISI index of certain type of bipartite graphs.

Theorem 3.7: Let G be a connected bipartite graph with bipartition $V(G) = V_1 \cup V_2$ such that $|V_1| = p$ and $|V_2| = q$. Let each of the partite sets V_i for $i = 1, 2$ has at least one dominating vertex. Then

$$\frac{pq}{p+q} + \frac{p(p-1)}{p+1} + \frac{q(q-1)}{q+1} \leq ISI(G) \leq \frac{p^2q^2}{p+p}.$$

Proof: Let $p + q = n$. The graph G has at least one vertex $v_1 \in V_1$ such that $deg_G(v_1) = q$ and at least one vertex $v_2 \in V_2$ such that $deg_G(v_2) = p$. The ISI matrix $A_{ISI}(G)$ has maximum number of nonzero entries if G has maximum of adjacencies. Since G is connected, the number of edges in G is at least $(n-1)$. The ISI index is minimum when G has $(n-1)$ edges and the partite sets V_1, V_2 have exactly one vertex of degree p, q, respectively. Further, G has the minimum ISI index when all other vertices of G has degree one, which means that the resultant graph is a bi-star graph on $(p+q)$ vertices. Thus the ISI index of G is the minimum when G is a bi-star graph. Thus from Theorem 3.4,

$$ISI(G) \leq \frac{pq}{p+q} + \frac{p(p-1)}{p+1} + \frac{q(q-1)}{q+1}.$$

In line with the similar argument, one can understand that the ISI index is the maximum when G has maximum number of edges and all the vertices have maximum possible degrees, that is, all the vertices are dominating. The graph G has the maximum ISI index when $deg_G(v_i) = p$ for all $v_i \in V_2$ and $deg_G(v_i) = p$ for all $v_i \in V_2$ and $deg_G(v_j) = q$ for all $v_i \in V_1$, that is $G = K_{p,q}$. Thus

$$ISI(G) \geq \frac{p^2q^2}{p+q}.$$

■

Next, we have a similar theorem which gives the bounds for ISI index, in the

Theorem 3.8: Let G be a connected graph of order n with the largest degree $\Delta(G) = n - 1$. Then

$$\frac{(n-1)^2}{n} \leq ISI(G) \leq \frac{n(n-1)^2}{4}.$$

Further, if $H = G^2$, then $ISI(H) = \frac{n(n-1)^2}{4}$.

Proof: Since $\Delta(G) = n-1$, there is at least one vertex in G whose degree is $(n-1)$. Without loss of generality, let v be the vertex which is adjacent with all the other vertices in G. For any vertex u in G, the entries corresponding to the vertex u, v is $\frac{deg_G(u) \times (n-1)}{deg_G(u)+(n-1)}$. Further, since the graph G is connected, $deg_G(u) \geq 1$. Thus

$$ISI(G) \geq (n-1) \times \frac{n-1}{n} = (n-1)^2.$$

■

Also, since $deg_G(u) \geq 1$,it follows that $ISI(G) \leq \frac{n(n-1)^2}{4}$. Due to the existence of the vertex v, for any vertices v_1, v_2 in G, the distance between v_1, v_2 is two due to the path $v_1 - v - v_2$. Hence every two vertices are adjacent in H and $H = K_n$. Thus

$$ISI(H) = \frac{n(n-1)^2}{4}.$$

Corollary 3.9: Let H_n be a helm graph and $G = H_n^2$. Then

$$\frac{4n^2}{2n+1} \leq ISI(G) \leq n^2(2n+1).$$

Proof: On noting that the graph G has $(2n+1)$ vertices and using Theorem 3.8, the result follows. ■

From Theorem 3.8, one can note that

$$ISI(H_n^3) = n^2(2n+1^2).$$

IV. Conclusion

The inverse sum in-degree is one of the degree-based topological indices, that has been explored by various molecular chemists in recent years. Squaring a graph is one of the classical operations on graphs that adds additional edges to the original graph based on certain conditions. The ISI index of graphs is obviously non-decreasing on squaring as the degree of the vertices either increases or remains unchanged. The ISI index of squares of graphs is derived for some classes. Also, the bounds for the ISI index of certain type of bipartite graphs are derived. The ISI index of some of the unexplored standard classes like fan graphs, friendship graphs, etc. are explored in this article.

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