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Study of inverse sum indeg index

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Abstract. Let $MG(i,n)$ $(1 \leq i \leq 3)$ denote to the class of all n-vertex molecular graphs with minimum degree i. The inverse sum indeg index of a graph is defined as $ISI = \sum_{uv \in E(G)} d_u d_v/(d_u + d_v)$, where d_u denotes to the degree of vertex u. In this paper, we propose some extremal molecular graphs with the minimum and the maximum value of inverse sum indeg index in $MG(i,n)$.

Keywords. inverse sum indeg index, molecular graphs, topological index.

1 Introduction

A graph G is called a molecular graph if the maximum degree of every vertex reaches to four, see [1]. Let $\sum = \{G : G \text{ is a finite simple graph}\}$, a topological index is a graph invariant $\eta : \sum \to \mathbb{R}^+$, that for two isomorphic graphs G and H, we have $\eta(G) = \eta(H)$. The **Wiener index** [2] is the first reported distance based topological index defined as half sum of the distances between all pair of vertices in a molecular graph. So far, many various types of topological indices have been described, see . [3–9]. One of the newest and the most efficient indices is the **inverse sum indeg index** (ISI index) defined as $ISI(G) = \sum_{uv \in E(G)} d_u d_v/(d_u + d_v)$, where d_u denotes the degree of vertex u. In this study, we determine those molecular graphs having the minimum and the maximum value of **ISI** index. For more information and new researches on this index, we refer the reader to [10,11] and the references therein.

Here, in the second section, we present the preliminary concepts and definitions which will be used in this paper. In the third section, we determine those molecular graphs having

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the extremal value of the *ISI* index among all molecular graphs with minimum degree i, where $i = 1,2,3$.

2 Definitions and Preliminaries

Let G be a molecular graph on n vertices and m edges. Let n_i denote the number of vertices with degree $i(i = 1,2,3,4)$ and x_{ij} be the number of edges connecting a vertex of degree i to a vertex of degree j. So, the ISI index of a molecular graph can be reformulated as follows:

$$ISI(G) = \sum_{1 \leq i \leq j \leq 4} \frac{ij}{i+j} x_{ij}. \tag{1}$$

Consider the set $X = \{1,2,\cdots,n\}$, a permutation group on X is a group Γ whose elements are permutations of X , namely bijective functions from X to X and whose group operation is the composition of permutations in Γ. The group of all permutations of X is called the symmetric group of X denoted by $Sym(X)$ or S_n, where X is finite and $n = |X|$. By this notation, a finite permutation group is a subgroup of the symmetric group S_n.

Let Aut(G) denote the automorphism group of the graph G. We say that Aut(G) acts transitively on $V(G)$, if for any pair of vertices $u,v \in V(G)$, there is $\alpha \in Aut(G)$ such that $\alpha(u) = v$. Similarly, Aut(G) acts transitively on $E(G)$, if for two arbitrary edges $e, f \in E(G)$, there is and automorphism $\alpha \in Aut(u)$ such that $\alpha(e) = f$.

Theorem 2.1. *Suppose G is an edge-transitive graph on m edges and $e = uv$ is an arbitrary edge. Then $ISI(G) = md_ud_v/(d_u + d_v)$. In particular, if G is k-regular, then $ISI(G) = mk/2 = m^2/n$.*

Proof. Clearly, since G is edge-transitive, for two edges $e = uv$ and $f = ab$, we have $\{d_u, d_v\} = \{d_a, d_b\}$. This completes the proof. □

Corollary 2.2. *Let G be a graph and $E_1(G), E_2(G), \cdots, E_s(G)$ be all orbits under the action of $Aut(G)$ on $E(G)$. Let $e_i = u_iv_i \in E_i(G)$, then*

$$ISI(G) = \sum_{i=1}^{s} |E_i(G)| \frac{d_{u_i} d_{v_i}}{d_{u_i} + d_{v_i}}.$$

Example 2.3. *Let S_n be the star graph on n vertices. It is a well-known fact that S_n is edge-transitive and so by Theorem2.1, $ISI(S_n) = m^2/n = (n-1)^2/n$.*

Example 2.4. *Consider the complete graph K_n. It is clear that K_n is edge-transitive and hence*

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

Example 2.5. *Suppose W_n denotes a wheel graph on n vertices, the action of $Aut(W_n)$ on edges has two orbits $E_1(W_n)$, $E_2(W_n)$, where $m_1 = |E_1(W_n)| = m_2 = |E_2(W_n)| = n-1$. For every edge*

$e_1 = u_1v_1 \in E_1(W_n)$, $d(u_1) = d(v_1) = 3$ and for every edge $e_2 = u_2v_2 \in E_2(W_n)$ and $d(u_2) = 3$, $d(v_2) = n-1$. Hence, by using Corollary 2.2, we have

$$ISI(W_n) = m_1\frac{3\cdot 3}{3+3} + m_2\cdot\frac{3(n-1)}{3+(n-1)} = \frac{9n(n-1)}{2(n+2)}.$$

Example 2.6. *Consider the path graph P_n on n vertices. It is not difficult to see that the number of orbits under the action Aut (P_n) on the vertices of P_n is*

$$\begin{cases} (n-1)/2 & n\equiv 1(mod2) \\ n/2 & n\equiv 0(mod2) \end{cases}.$$

Further, if n is odd, then each orbit under the action of Aut (P_n) on edges is of order 2 and if n is even, then P_n has $(n/2)-1$ orbits of order 2 and a singleton orbit (an orbit of size one). Hence, for $n \geqslant 3$, by using Corollary 2.2, we have $ISI(P_n) = n - 5/3$.

3 Main Results

Let $MG(i,n)$, denote all connected molecular graphs with n vertices and minimum degree i, where $i = 1,2,3$. The aim of this section is to compute the extremal graphs for ISI index in class $MG(i,n)$.

3.1 Extremal molecular graphs in $MG(1,n)$

First, we propose the extremal molecular graphs with respect to ISI index in $MG(1,n)$. In [10] the authors proved that for $n \leqslant 5$, the star graph S_n has the minimum value of ISI index and for $n \geqslant 6$, the path P_n has the minimum value of ISI index among all molecular graphs. For the maximum value of ISI index, by considering $Eq.(1)$ and substituting the term $a_{ij} = \dfrac{ij}{i+j}$ in ISI index, we have:

$$ISI(G) = a_{11}x_{11} + a_{12}x_{12} + a_{13}x_{13} + a_{14}x_{114} + x_{22} + a_{23}x_{23} + a_{24}x_{24} + a_{33}x_{33} + a_{34}x_{34} + 2x_{44}.$$

It is clear that for $n \geqslant 5$ a 4-regular molecular graph has the maximum ISI index, but in class $MG(1,n)$ there is at least a vertex of degree 1. Suppose $n_1 = 1$, and the other vertices are of degree four, then the summation of vertex degrees is then $4n-3$ which is an odd number, a contradiction with Eulers formula. So we can suppose that $n_2 \neq 0$ or $n_3 \neq 0$. First notice than the maximum value of

$$f(x,y) = \frac{xy}{x+y}, 1 \leq x,y \leq 4 \tag{2}$$

holds for $x = y = 4$ and thus $f(4,4) = 2$. Since, $1 \leq x,y \leq 4$ we have $f(x,y) \leq 2$, it is clear that a graph with maximum ISI index in $MG(1,n)$ has the maximum number of both vertices of degree 4 and possible edges. In other word, if $H \in MG(1,n)$ has the maximum ISI index, then H has $(n-2)$ vertices of degree 4, a vertex of degree 1 and a vertex of degree 2 or 3. According to Eulers theorem, a graph with degree sequence $1,2,4,\underbrace{...}_{n-2},4$ does not exist. Hence, H has a vertex of degree 3 and we can consider two following cases:

- the pendant edge is added to a vertex of degree three. In this case. In this case, the ISI index of H is $4n - 163/28$.
- The pendant edge is added to a vertex of degree four. In this case, the ISI index of H is $4n - 212/35$.

  Comparing these values implies that the graph H depicted in Figure 1 has the maximum value of ISI index in $MG(1,n)$ and thus we can conclude the following theorem.

Theorem 3.1. *Among all n-vertex molecular graphs having minimum degree 1, we have:*

- *If $n \leq 5$ then S_n has the minimum value of ISI index and if $n \geq 6$, P_n has the minimum value, see [10].*
- *For $n \geq 7$, a molecular graph with a single vertex of degree three adjacent to a vertex of degree one and the other vertices of degree four is one with the maximum ISI index. This molecular graph is unique, see Figure 1.*

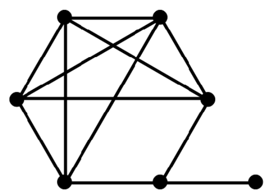

Figure 1. Molecular graph H with maximum ISI index in $MG(1,n)$ for $n = 7$.

3.2 Extremal molecular graphs in $MG(2,n)$

Here, we determine those molecular graphs having the minimum and the maximum value of ISI index in $MG(2,n)$. Regarding $a_{ij} = ij/(i+j)$, the value of ISI index can be calculated as follows:

$$ISI(G) = x_{22} + a_{23}x_{23} + a_{24}x_{24} + a_{33}x_{33} + a_{34}x_{34} + 2x_{44}.$$

In finding a molecular graph with the minimum value of ISI index in $MG(2,n)$, by using $Eq.(2)$ we have:

$$x_{22} = n - 5x_{23}/6 - 3x_{24}/4 - 2x_{33}/3 - 7x_{34}/12 - x_{44}/2.$$

Now, by replacing x_{22} in $Eq.(3)$, we obtain:

$$ISI(G) = n + (a_{23} - 5/6)x_{23} + (a_{24} - 3/4)x_{24} + (a_{33} - 2/3)x_{33} + (a_{34} - 7/12)x_{34} + 3x_{44}/2.$$

By a simple calculation, we can see that all terms $x_{44}, x_{34}, x_{33}, x_{24}, x_{23}$ are positive. Clearly, for every $n \geq 3$, the molecular graph G with $n_2 = n$ and $x_{22} = n$, is one with the minimum value of ISI index. In other words, let G be a molecular graph on n vertices, where $n_2 \leq n-1$, hence G has at least two vertices of degree greater than 2. For example, suppose G has two vertices of degree 3 and the other vertices are of degree two, then $ISI(G) = n + 23/10$ which is greater than $ISI(C_n)$. It is obvious that the cycle C_n has the minimum both edges and vertex degrees among all graphs on n vertices. This yields that if G has vertices of degree greater than two then $ISI(G)ISI(C_n) = n$ and so C_n is the unique molecular graph with the minimum ISI index.

For finding a graph with maximum ISI index in $MG(2,n)$, since a 4-regular graph has the maximum value of ISI among all connected graphs, similar to the proof of Theorem 3.1, the extremal graph in the class $MG(2,n)$ certainly has the maximum number of vertices of degree 4. Suppose G has $(n-1)$ vertices of degree 4 and a vertex of degree 2 or 3. In the first case we construct a graph with $ISI(G) = 4n - 10/3$. In the second case, there is no graph by these conditions. In other words, we proved the following theorem:

Theorem 3.2. *Among all n-vertex molecular graphs with minimum degree 2, we have:*

- *For $n \geq 3$, cycle C_n has the minimum value of ISI index.*
- *For $n \geq 6$, a molecular graph G with a single vertex of degree two and the other vertices of degree four is one with the maximum value of ISI index in which $ISI(G) = 4n - 10/3$.*

3.3 Extremal graphs in $MG(3,n)$

Here, we determine those molecular graphs with the minimum and maximum values of ISI index in $MG(3,n)$. First suppose n is even. It is clear that a graph with the minimum value of ISI index has the maximum possible vertices of degree three with minimum edges, since for the function $f(x,y) = xy/(x+y)$, we have $f(3,3) = 3/2$ and $f(3,4) = 12/7$. Clearly if all vertices are of degree three then we have both minimum number of edges and minimum value of $f(x,y)$. This yields that the graph G depicted in Figure 2 has the minimum ISI index which is equal $9n/4$. If n is odd then at least one of vertices should be of degree four and our computation shows that $ISI(G) = 9n/4 + 45/28$. By a similar method we can prove that a graph G belong to $MG(3,n)$ has the maximum value of ISI index if it has maximum number of vertices of degree four which is $n-2$ and thus we have two vertices of degree three. Two cases hold:

- two vertices of degree three are not adjacent. By a direct computation we have $ISI(G) = 4n - 26/7$.
- Two vertices of degree three are adjacent and then $ISI(G) = 4n - 51/14$.

So, we proved the following theorem.

Theorem 3.3. *Among all n-vertex molecular graphs with minimum degree 3, we have*

- *If $n \equiv 1 \pmod 2$, then for $n \geq 5$, a molecular graph with a single vertex of degree four adjacent to four vertices of degree three and the other edges connect the vertex of degree three to a vertex of degree three, is a molecular graph with the minimum value of ISI index which is equal to $9n/4 + 45/28$. Note that this molecular graph is not unique, see Figure 2.*

- *If $n \equiv 0 \pmod 2$, then for $n \geq 6$, a molecular graph with two vertices of degree four, each of them adjacent to four vertices of degree three, and the other edges connect a vertex of degree three to a vertex of degree three, is a molecular graph that possesses the minimum value of ISI index and this value is equal to $9n/4$. Note that this molecular graph is not unique, see Figure 3.*

- *For $n \geq 6$, a molecular graph with two adjacent vertices of degree three and the other vertices of degree four is a molecular graph that possesses the maximum values of ISI index and this value is equal to $4n - 51/14$. Note that this molecular graph is not unique, see Figure 4.*

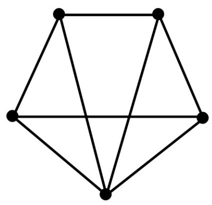

Figure 2. Molecular graph with minimum ISI index in $MG(3,n)$(n is odd) for $n = 5$.

Figure 3. Molecular graph with minimum (left hand) and maximum (right hand) ISI index in $MG(3,n)$ for $n = 6$.

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