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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
Mathematics Subject Classification (2010): 05C09.

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

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will be used in this paper. In the third section, we determine those molecular graphs having 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 Euler鈥檚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 Euler鈥檚theorem, a graph with degree sequence $1,2,4,\underbrace{\dots}_{n-2},4$ 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.*

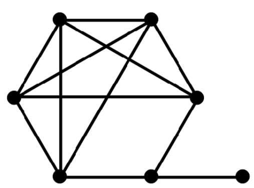

Figure 1. Molecular graph H with maximum ISI index in $MG(1,n)$ for $n=7$.

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 $ISI(G)FSI(C_n) = n$ 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.*

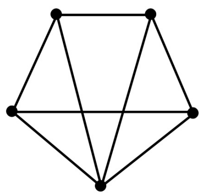

Figure 2. Molecular graph with minimum ISI index in $MG(3,n)$(n is odd) for $n = 5$.

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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