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On Relations Between Inverse Sum Indeg Index and Multiplicative Sum Zagreb Index

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Abstract: In this paper we derive some lower and upper bounds for the inverse sum indeg index, $ISI = \sum_{i\sim j} \frac{d_i d_j}{d_i + d_j}$, in terms of graph invariants $F = \sum_{i=1}^{n} d_i^3$ and $\Pi_1^* = \prod_{i\sim j}(d_i + d_j)$.

Keywords: Vertex degree, inverse sum indeg index, multiplicative sum Zagreb index.

1 Introduction

Let $G = (V,E)$, $V = \{1,2,\ldots,n\}$, $E = \{e_1,e_2,\ldots,e_m\}$, be a simple connected graph and $d_1 \geq d_2 \geq \cdots \geq d_n > 0$, $d_i = d(i)$, and $d(e_1) \geq \cdots \geq d(e_m)$ its sequences of vertex and edge degrees, respectively. Throughout the paper we use the following notation: $\Delta_{e_1} = d(e_1)+2$, $\Delta_{e_2} = d(e_2)+2$, $\delta_{e_1} = d(e_m)+2$, and $\delta_{e_2} = d(e_{m-1})+2$. With $i \sim j$ $(i,j \in V)$ we denote the adjacency of vertices i and j in G.

Two vertex-degree based topological indices, the first and the second Zagreb index, M_1 and M_2, are defined as [7]

$$M_1 = M_1(G) = \sum_{i=1}^{n} d_i^2 \quad \text{and} \quad M_2 = M_2(G) = \sum_{i\sim j} d_i d_j .$$

As shown in [11, 12], the first Zagreb index can be also expressed as

$$M_1 = \sum_{i\sim j}(d_i + d_j) = \sum_{i=1}^{m}(d(e_i)+2).$$

A so-called forgotten topological index, F, is defined as [7] (see also [6])

$$F = F(G) = \sum_{i=1}^{n} d_i^3 = \sum_{i\sim j}(d_i^2 + d_j^2).$$

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By analogy to M_1, the invariant F can be written in the following way

$$F = \sum_{i=1}^{m} (d(e_i)+2)^2 - 2M_2 .$$

Multiplicative versions of topological indices were proposed in 2010 [15], whereas the first and second multiplicative Zagreb indices were first considered in a paper [9] published in 2011, and were promptly followed by numerous additional studies. One year later, the multiplicative sum–Zagreb index, Π_1^*, was introduced [4]:

$$\Pi_1^* = \Pi_1^*(G) = \prod_{i \sim j} (d_i + d_j).$$

It is not difficult to see that this topological index can be also considered as an edge–degree–based topological index, i.e. that the following equality is valid

$$\Pi_1^* = \prod_{i=1}^{m} (d(e_i)+2).$$

A family of Adriatic indices was introduced in [16, 17]. An especially interesting subclass of these descriptors consists of 148 discrete Adriatic indices. A so called inverse sum indeg index, *ISI*, was selected in [17] as a significant predictor of total surface area of octane isomers. The inverse indeg index is defined as

$$ISI = ISI(G) = \sum_{i \sim j} \frac{d_i d_j}{d_i + d_j}.$$

For more details on this topological index see, for example, in [5, 13].

In this paper we determine lower and upper bounds for *ISI* in terms of invariants F and Π_1^*, and some of the graph parameters m, Δ_{e_1}, Δ_{e_2}, δ_{e_1}, and δ_{e_2}.

2 Preliminaries

In this section we list some analytic inequalities for real number sequences that will be used in the subsequent considerations.

Let $a = (a_i)$, and $b = (b_i)$, $i = 1, 2, \ldots, m$, be two positive real number sequences with the properties

$$0 < r_1 \le a_i \le R_1 < +\infty \quad \text{and} \quad 0 < r_2 \le b_i \le R_2 < +\infty.$$

In [1] the following inequality was proven

$$\left| m \sum_{i=1}^{m} a_i b_i - \sum_{i=1}^{m} a_i \sum_{i=1}^{m} b_i \right| \le m^2 \alpha(m)(R_1 - r_1)(R_2 - r_2), \tag{1}$$

where

$$\alpha(m) = \frac{1}{4}\left(1 - \frac{(-1)^{m+1}+1}{2m^2}\right).$$

Let $a = (a_i)$, $i = 1, 2, \ldots, m$, be positive real number sequence. In [18] (see also [10]) it was proven

$$\left(\sum_{i=1}^{m} \sqrt{a_i}\right)^2 \le (m-1)\sum_{i=1}^{m} a_i + m\left(\prod_{i=1}^{m} a_i\right)^{\frac{1}{m}}. \tag{2}$$

Let $a = (a_i)$, $i = 1, 2, \ldots, m$, be positive real number sequence with the property $0 < r \le a_i \le R < +\infty$. Szőkefalvi Nagy [14] proved that

$$m\sum_{i=1}^{m} a_i^2 - \left(\sum_{i=1}^{m} a_i\right)^2 \ge \frac{m}{2}(R-r)^2. \tag{3}$$

3 Main results

The following theorem establishes an upper bound for the *ISI* in terms of invariants F and Π_1^*, and parameters m, Δ_{e_1}, Δ_{e_2}, and δ_{e_1}.

Theorem 3.1. *Let G be a simple connected graph with $m \ge 2$ edges. Then*

$$ISI \le \frac{1}{2\delta_{e_1}}\left(\Delta_{e_1}^2 + (m-1)\left(\frac{\Pi_1^*}{\Delta_{e_1}}\right)^{\frac{2}{m-1}} - F + (m-1)^2\alpha(m-1)(\Delta_{e_2} - \delta_{e_1})^2\right). \tag{4}$$

Equality holds if and only if $\Delta_{e_2} = d(e_2) + 2 = \cdots = d(e_m) + 2 = \delta_{e_1}$.

Proof. The inequality (1) can be written as

$$\left|(m-1)\sum_{i=2}^{m} a_i b_i - \sum_{i=2}^{m} a_i \sum_{i=2}^{m} b_i\right| \le (m-1)^2\alpha(m-1)(R_1 - r_1)(R_2 - r_2).$$

For $a_i = b_i = d(e_i) + 2$, $i = 2, \ldots, m$, $R_1 = \Delta_{e_2}$, $r_1 = \delta_{e_1}$, this inequality becomes

$$(m-1)\sum_{i=2}^{m}(d(e_i)+2)^2 - \left(\sum_{i=2}^{m}(d(e_i)+2)\right)^2 \le (m-1)^2\alpha(m-1)(\Delta_{e_2} - \delta_{e_1})^2. \tag{5}$$

The inequality (2) can be expressed as

$$\left(\sum_{i=2}^{m} \sqrt{a_i}\right)^2 \le (m-2)\sum_{i=2}^{m} a_i + (m-1)\left(\prod_{i=2}^{m} a_i\right)^{\frac{1}{m-1}}.$$

Setting $a_i = (d(e_i)+2)^2$, $i = 2,\ldots,m$, in the above inequality, we get

$$\left(\sum_{i=2}^{m}(d(e_i)+2)\right)^2 \leq (m-2)\sum_{i=2}^{m}(d(e_i)+2)^2 + (m-1)\left(\prod_{i=2}^{m}(d(e_i)+2)^2\right)^{\frac{1}{m-1}}. \quad (6)$$

From (5) and (6) follows

$$\sum_{i=2}^{m}(d(e_i)+2)^2 \leq (m-1)\left(\prod_{i=2}^{m}(d(e_i)+2)^2\right)^{\frac{1}{m-1}} + (m-1)^2\alpha(m-1)(\Delta_{e_2}-\delta_{e_1})^2,$$

i.e.

$$F + 2M_2 \leq \Delta_{e_1}^2 + (m-1)\left(\frac{\Pi_1^*}{\Delta_{e_1}}\right)^{\frac{2}{m-1}} + (m-1)^2\alpha(m-1)(\Delta_{e_2}-\delta_{e_1})^2. \quad (7)$$

According to the inequalities

$$\frac{1}{\Delta_{e_1}}\sum_{i\sim j} d_i d_j \leq \sum_{i\sim j}\frac{d_i d_j}{d_i+d_j} \leq \frac{1}{\delta_{e_1}}\sum_{i\sim j} d_i d_j,$$

we have

$$\frac{M_2}{\Delta_{e_1}} \leq ISI \leq \frac{M_2}{\delta_{e_1}}. \quad (8)$$

The inequality (4) is obtained from (7) and right inequality in (8).

□

Since $\alpha(m) \leq \frac{1}{4}$, $\Delta_{e_2} \leq \Delta_{e_1} \leq 2\Delta$, $\delta_{e_1} \geq 2\delta$, we have the following corollary of Theorem 3.1.

Corollary 3.2. *Let G be a simple connected graph with $n \geq 3$ vertices and m edges. Then*

$$ISI \leq \frac{1}{4\delta}\left(4\Delta^2 + (m-1)\left(\frac{\Pi_1^*}{2\delta}\right)^{\frac{2}{m-1}} - F + (m-1)^2(\Delta-\delta)^2\right).$$

Equality holds if and only if G is a regular graph.

By a similar procedure as in the case of Theorem 3.1, the following statements can be proved.

Theorem 3.3. *Let G be a simple connected graph with $m \geq 2$ edges. Then*

$$ISI \leq \frac{1}{2\delta_{e_1}}\left(\delta_{e_1}^2 + (m-1)\left(\frac{\Pi_1^*}{\delta_{e_1}}\right)^{\frac{2}{m-1}} - F + (m-1)^2\alpha(m-1)(\Delta_{e_1}-\delta_{e_2})^2\right).$$

Equality holds if and only if $\Delta_{e_1} = d(e_1)+2 = \cdots = d(e_{m-1})+2 = \delta_{e_2}$.

Theorem 3.4. *Let G be a simple connected graph with* $m \geq 3$ *edges. Then*

$$ISI \leq \frac{1}{2\delta_{e_1}} \left(\Delta_{e_1}^2 + \delta_{e_1}^2 + (m-2) \left(\frac{\Pi_1^*}{\Delta_{e_1}\delta_{e_1}} \right)^{\frac{2}{m-2}} - F \right.$$
$$\left. + (m-2)^2 \alpha(m-2)(\Delta_{e_2} - \delta_{e_2})^2 \right).$$

Equality holds if and only if $\Delta_{e_2} = d(e_2) + 2 = \cdots = d(e_{m-1}) + 2 = \delta_{e_2}$.

In the next theorem we determine lower bound for the *ISI* in terms of F and Π_1^*, and graph parameters m, Δ_{e_1}, Δ_{e_2}, δ_{e_1}, and δ_{e_2}.

Theorem 3.5. *Let G be a simple connected graph with m,* $m \geq 2$*, edges. Then*

$$ISI \geq \frac{1}{2\Delta_{e_1}} \left(\Delta_{e_1}^2 + (m-1) \left(\frac{\Pi_1^*}{\Delta_{e_1}} \right)^{\frac{2}{m-1}} - F + \frac{1}{2}(\Delta_{e_2} - \delta_{e_1})^2 \right). \tag{9}$$

Equality holds if and only if $\Delta_{e_2} = d(e_2) + 2 = \cdots = d(e_m) + 2 = \delta_{e_1}$.

Proof. The inequality (3) will be considered as

$$(m-1)\sum_{i=2}^{m} a_i^2 - \left(\sum_{i=2}^{m} a_i \right)^2 \geq \frac{m-1}{2}(R-r)^2.$$

For $a_i = d(e_i) + 2$, $i = 2, \ldots, m$, $R = \Delta_{e_2} = d(e_2) + 2$ and $r = \delta_{e_1} = d(e_m) + 2$, the above inequality becomes

$$(m-1)\sum_{i=2}^{m} (d(e_i)+2)^2 - \left(\sum_{i=2}^{m} (d(e_i)+2) \right)^2 \geq \frac{m-1}{2}(\Delta_{e_2} - \delta_{e_1})^2. \tag{10}$$

Using the arithmetic-geometric mean inequality, we get

$$\left(\sum_{i=2}^{m} (d(e_i)+2) \right)^2 \geq (m-1)^2 \left(\prod_{i=2}^{m} (d(e_i)+2) \right)^{\frac{2}{m-1}},$$

i.e.

$$\left(\sum_{i=2}^{m} (d(e_i)+2) \right)^2 \geq (m-1)^2 \left(\frac{\Pi_1^*}{\Delta_{e_1}} \right)^{\frac{2}{m-1}}. \tag{11}$$

From (10) and (11) follows

$$(m-1)\sum_{i=2}^{m} (d(e_i)+2)^2 \geq (m-1)^2 \left(\frac{\Pi_1^*}{\Delta_{e_1}} \right)^{\frac{2}{m-1}} + \frac{m-1}{2}(\Delta_{e_2} - \delta_{e_1})^2,$$

i.e.

$$F+2M_2 \geq \Delta_{e_1}^2+(m-1)\left(\frac{\Pi_1^*}{\Delta_{e_1}}\right)^{\frac{2}{m-1}}+\frac{1}{2}(\Delta_{e_2}-\delta_{e_1})^2.$$

According to this inequality and left inequality in (8) we obtain (9).

□

By a similar procedure as in case of Theorem 3.5, the following theorems can be proved.

Theorem 3.6. *Let G be a simple connected graph with $m \geq 2$ edges. Then*

$$ISI \geq \frac{1}{2\Delta_{e_1}}\left(\delta_{e_1}^2+(m-1)\left(\frac{\Pi_1^*}{\delta_{e_1}}\right)^{\frac{2}{m-1}}-F+\frac{1}{2}(\Delta_{e_1}-\delta_{e_2})^2\right).$$

Equality holds if and only if $\Delta_{e_1}=d(e_1)+2=\cdots=d(e_{m-1})+2=\delta_{e_2}$.

Theorem 3.7. *Let G be a simple connected graph with $m \geq 3$ edges. Then*

$$ISI \geq \frac{1}{2\Delta_{e_1}}\left(\Delta_{e_1}^2+\delta_{e_1}^2+(m-2)\left(\frac{\Pi_1^*}{\Delta_{e_1}\delta_{e_1}}\right)^{\frac{2}{m-2}}-F+\frac{1}{2}(\Delta_{e_2}-\delta_{e_2})^2\right).$$

Equality holds if and only if $\Delta_{e_2}=d(e_2)+2=\cdots=d(e_{m-1})+2=\delta_{e_2}$.

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