



Some new upper bounds for the inverse sum indeg index of graphs

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Abstract

Let $G = (V, E)$ be a simple connected graph with the vertex set $V = \{1, 2, \dots, n\}$ and sequence of vertex degrees (d_1, d_2, \dots, d_n) where d_i denotes the degree of a vertex $i \in V$. With $i \sim j$, we denote the adjacency of the vertices i and j in the graph G . The inverse sum indeg (ISI) index of the graph G is defined as $ISI(G) = \sum_{i \sim j} \frac{d_i d_j}{d_i + d_j}$. Some new upper bounds for the ISI index are obtained in this paper.

Keywords: vertex-degree-based topological indices, inverse sum indeg index, Zagreb indices, multiplicative Zagreb indices.

Mathematics Subject Classification: 05C07; 05C35; 92E10

DOI: 10.5614/ejgta.2020.8.1.5

1. Introduction

Let G be a simple connected graph with the vertex set $V = \{1, 2, \dots, n\}$, edge set $E = \{e_1, e_2, \dots, e_m\}$ and sequence of vertex degrees (d_1, d_2, \dots, d_n) satisfying $d_1 \geq d_2 \geq \dots \geq d_n > 0$ where d_i is the degree of a vertex $i \in V$. If $e \in E$ is an edge connecting the vertices i and j , then degree of the edge e is defined as $d(e) = d_i + d_j - 2$. Denote by $(d(e_1), d(e_2), \dots, d(e_m))$ the sequence of edge degrees satisfying $d(e_1) \geq d(e_2) \geq \dots \geq d(e_m)$. As usual, we assume that $\Delta = d_1 \geq d_2 \geq \dots \geq d_n = \delta > 0$ and $\Delta_e = d(e_1) + 2 \geq d(e_2) + 2 \geq \dots \geq d(e_m) + 2 = \delta_e$. If the vertices i and j are adjacent, we write $i \sim j$.

Received: 19 May 2018, Revised: 12 June 2019, Accepted: 26 October 2019.

In graph theory, an invariant is a numerical quantity of graphs that depends only on their abstract structure, not on the labeling of vertices or edges, or on the drawing of the graphs. In chemical graph theory, such quantities are also referred to as topological indices. Topological indices gained considerable popularity because of their applications in chemistry as molecular structure descriptors [10, 32, 33].

A large number of topological indices have been derived depending on vertex degrees. Among the oldest are the first and the second Zagreb index, M_1 and M_2 , defined as [17, 18]

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

As shown in [26], the first Zagreb index can be written as

$$M_1 = \sum_{i \sim j} (d_i + d_j).$$

Bearing in mind that for the edge e connecting the vertices i and j , holds

$$d(e) = d_i + d_j - 2,$$

the index M_1 can also be considered as an edge-degree-based topological index [23, 24]

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

The following multiplicative variants of the first and the second Zagreb indices, Π_1 and Π_2 , were introduced in [19] (see also [34])

$$\Pi_1 = \Pi_1(G) = \prod_{i=1}^n d_i^2 \quad \text{and} \quad \Pi_2 = \Pi_2(G) = \prod_{i \sim j} d_i d_j.$$

Soon after the appearance of Π_1 and Π_2 , the multiplicative sum Zagreb index, Π_1^* , was introduced [11]

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

The sum-connectivity index, SCI , is defined as [36]

$$SCI = SCI(G) = \sum_{i \sim j} \frac{1}{\sqrt{d_i + d_j}}.$$

Probably the most popular and most thoroughly investigated molecular-structure descriptor is the classical Randić (or connectivity) index

$$R = R(G) = \sum_{i \sim j} \frac{1}{\sqrt{d_i d_j}},$$

defined in [29]. The general Randić index, R_α , is defined [6] as

$$R_\alpha = R_\alpha(G) = \sum_{i \sim j} (d_i d_j)^\alpha,$$

where α is a non-zero real number. Here we are interested in the case $\alpha = -1$, that is for R_{-1} . This was defined in [26] under the name modified second Zagreb index.

The harmonic index, H , is defined as [12]

$$H = H(G) = \sum_{i \sim j} \frac{2}{d_i + d_j}.$$

Details about the mathematical properties of all the above mentioned topological indices can be found in the surveys [2, 3, 7, 14, 20, 21] and related references listed therein. Here, it needs to be mentioned that the Harary index [9] is also denoted by H – but in the remaining part of this paper, by the notation H , we mean the harmonic index.

A family of 148 discrete Adriatic indices was introduced and analyzed in [35]. An especially interesting subclass of these 148 topological indices consists of 20 indices, which are useful for predicting the certain physicochemical properties of chemical compounds. The so called inverse sum indeg (ISI) index is one of these 20 indices. It is defined as

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

The ISI index is a significant predictor of total surface area for octane isomers [35]. The problem of finding bounds on the ISI index has gained a considerable attention from researchers in recent years, for example, see [4, 5, 8, 13, 15, 16, 22, 27, 31]. In this paper, we derive several new upper bounds on the ISI index in terms of some graph parameters and above mentioned vertex–degree–based topological indices.

2. Preliminaries

In this section, we recall some discrete inequalities for real number sequences that will be used in the subsequent considerations.

Let $p = (p_k)$ and $a = (a_k)$, $k = 1, 2, \dots, m$, be two positive real number sequences with the properties $p_1 + p_2 + \dots + p_m = 1$ and $0 < r \leq a_k \leq R < +\infty$. In [30], the following inequality was proven

$$\sum_{k=1}^m p_k a_k + rR \sum_{k=1}^m \frac{p_k}{a_k} \leq r + R. \tag{1}$$

Equality in (1) holds if and only if either $R = a_1 = \dots = a_m = r$ or $R = a_1 = \dots = a_s \geq a_{s+1} = \dots = a_m = r$ for some s , $1 \leq s \leq m - 1$.

Let $a = (a_k)$ and $b = (b_k)$, $k = 1, 2, \dots, m$, be positive real number sequences. In [28], it was proven that for any $r \geq 0$, it holds

$$\sum_{k=1}^m \frac{a_k^{r+1}}{b_k^r} \geq \frac{\left(\sum_{k=1}^m a_k\right)^{r+1}}{\left(\sum_{k=1}^m b_k\right)^r}, \tag{2}$$

with equality if and only if $\frac{a_1}{b_1} = \frac{a_2}{b_2} = \dots = \frac{a_m}{b_m}$.

3. Main results

In the following theorem, we established an upper bound for the inverse sum indeg index, in terms of graph parameters n , Δ_e and δ_e and topological indices M_1 and M_2 .

Theorem 3.1. *If G is a simple connected graph with $n \geq 2$ vertices then*

$$ISI \leq \frac{n(\Delta_e + \delta_e)M_2 - M_1^2}{n\Delta_e\delta_e}. \tag{3}$$

Equality sign in (3) holds if and only if G is regular or semiregular bipartite graph.

Proof. For $p_k := \frac{d_i d_j}{\sum_{i \sim j} d_i d_j}$, $a_k := d_i + d_j$, $r = \delta_e$, $R = \Delta_e$, where summation is performed over all edges in graph G , the inequality (1) becomes

$$\frac{\sum_{i \sim j} d_i d_j (d_i + d_j)}{\sum_{i \sim j} d_i d_j} + \frac{\Delta_e \delta_e \sum_{i \sim j} \frac{d_i d_j}{d_i + d_j}}{\sum_{i \sim j} d_i d_j} \leq \Delta_e + \delta_e,$$

that is

$$\sum_{i \sim j} d_i d_j (d_i + d_j) + \Delta_e \delta_e ISI \leq (\Delta_e + \delta_e)M_2. \tag{4}$$

For $r = 1$, $a_k := d_i + d_j$, $b_k := \frac{1}{d_i} + \frac{1}{d_j}$, where summation is performed over all edges in G , the inequality (2) becomes

$$\sum_{i \sim j} \frac{(d_i + d_j)^2}{\frac{1}{d_i} + \frac{1}{d_j}} \geq \frac{\left(\sum_{i \sim j} (d_i + d_j)\right)^2}{\sum_{i \sim j} \left(\frac{1}{d_i} + \frac{1}{d_j}\right)},$$

i.e.

$$\sum_{i \sim j} d_i d_j (d_i + d_j) \geq \frac{M_1^2}{n}. \tag{5}$$

According to (4) and (5) follows

$$\frac{M_1^2}{n} + \Delta_e \delta_e ISI \leq (\Delta_e + \delta_e) M_2, \tag{6}$$

wherefrom we obtain (3).

Equality in (1) holds if and only if either $a_1 = a_2 = \dots = a_m$, or $a_1 = a_2 = \dots = a_s \geq a_{s+1} = \dots = a_m$ for some $s, 1 \leq s \leq m - 1$. This means that equality in (4) is attained if and only if either $\Delta_e = d(e_1) + 2 = \dots = d(e_m) + 2 = \delta_e$, or $\Delta_e = d(e_1) + 2 = \dots = d(e_s) + 2 \geq d(e_{s+1}) + 2 = \dots = d(e_m) + 2 = \delta_e$ for some $s, 1 \leq s \leq m - 1$. Equality in (2) holds if and only if $\frac{a_1}{b_1} = \frac{a_2}{b_2} = \dots = \frac{a_m}{b_m}$, therefore equality in (5) holds if and only if $d_i d_j = c, c = \text{constant}$, for every edge of G . Let j and v be two vertices adjacent to i , that is $i \sim j$ and $i \sim v$. Then, it holds $d_i d_j = d_i d_v$, i.e. $d_j = d_v$. This implies that equality in (5) holds if and only if G is regular or semiregular bipartite graph. Finally, we conclude that equality in (3) holds if and only if G is regular or semiregular bipartite graph. \square

Corollary 3.1. *If G is a simple connected graph with $n \geq 2$ vertices then*

$$ISI \leq \frac{n(\Delta_e + \delta_e)^2 M_2^2}{4\Delta_e \delta_e M_1^2} \leq \frac{n(\Delta + \delta)^2 M_2^2}{4\Delta \delta M_1^2}. \tag{7}$$

The equality sign in the first inequality holds if and only if G is regular or semiregular bipartite graph. Equality in the second inequality holds if and only if $\delta_e = 2\delta$ and $\Delta_e = 2\Delta$.

Proof. Using the arithmetic-geometric mean inequality for real numbers (see e.g. [25]), according to (6) we get

$$2\sqrt{\frac{\Delta_e \delta_e M_1^2 ISI}{n}} \leq \frac{M_1^2}{n} + \Delta_e \delta_e ISI \leq (\Delta_e + \delta_e) M_2,$$

wherefrom we obtain the first inequality in (7).

The second inequality in (7) follows from the first inequality and from the following inequality

$$2\delta \leq \delta_e \leq \Delta_e \leq 2\Delta.$$

\square

In the next theorem, we derive an upper bound for the ISI index in terms of the graph parameters m, Δ_e, δ_e and topological indices R, H and M_2 .

Theorem 3.2. *If G is a simple connected graph with $m \geq 1$ edges then*

$$ISI \leq \frac{(\Delta_e + \delta_e) R^2 H M_2 - 2m^4}{\Delta_e \delta_e R^2 H}. \tag{8}$$

Equality holds if and only if G is regular or semiregular bipartite graph.

Proof. For $r = 1$, $a_k := \sqrt{d_i d_j}$, $b_k := \frac{1}{d_i + d_j}$, where summation is performed over all edges in G , the inequality (2) becomes

$$\sum_{i \sim j} d_i d_j (d_i + d_j) = \sum_{i \sim j} \frac{(\sqrt{d_i d_j})^2}{\frac{1}{d_i + d_j}} \geq \frac{\left(\sum_{i \sim j} \sqrt{d_i d_j}\right)^2}{\sum_{i \sim j} \frac{1}{d_i + d_j}},$$

that is

$$\sum_{i \sim j} d_i d_j (d_i + d_j) \geq \frac{2 \left(\sum_{i \sim j} \sqrt{d_i d_j}\right)^2}{H}. \tag{9}$$

Using the arithmetic-harmonic mean inequality for real numbers (see [25]), we have that

$$\left(\sum_{i \sim j} \sqrt{d_i d_j}\right) \left(\sum_{i \sim j} \frac{1}{\sqrt{d_i d_j}}\right) \geq m^2,$$

i.e.

$$\left(\sum_{i \sim j} \sqrt{d_i d_j}\right)^2 \geq \frac{m^4}{R^2}. \tag{10}$$

From (9) and (10), it follows that

$$\sum_{i \sim j} d_i d_j (d_i + d_j) \geq \frac{2m^4}{HR^2}. \tag{11}$$

Finally, from (11) and (4), the desired inequality follows.

Equality in (9) holds if and only if $d_i d_j (d_i + d_j) = c$, $c = const.$, for every edge of G . Equality in (10) holds if and only if $d_i d_j = c_1$, $c_1 = constant$, for every edge of G . Let j and v be two vertices adjacent to vertex i , that is $i \sim j$ and $i \sim v$. Then, equalities in (9) and (10) hold if and only if $d_j = d_v$. Since the graph G is connected, equalities in (9) and (10) hold if and only if G is regular or semiregular bipartite graph. Therefore, equality in (11) holds if and only if G is regular or semiregular bipartite graph. Equalities in both (4) and (11) hold if and only if G is regular or semiregular bipartite graph. Finally, equality in (8) holds if and only if G is regular or semiregular bipartite graph. \square

By the similar arguments as in case of Corollary 3.1, the following corollary of Theorem 3.2 can be proved.

Corollary 3.2. *Let G be a simple connected graph with $m \geq 1$ edges. Then*

$$ISI \leq \frac{(\Delta_e + \delta_e)^2 HR^2 M_2^2}{8\Delta_e \delta_e m^4} \leq \frac{(\Delta + \delta)^2 HR^2 M_2^2}{8\Delta \delta m^4}.$$

Equality in the first inequality holds if and only if G is regular or semiregular bipartite graph. Equality in the second inequality holds if and only if $\delta_e = 2\delta$ and $\Delta_e = 2\Delta$.

In the following theorem, we establish an upper bound for the *ISI* index in terms of parameters m , Δ_e , δ_e and topological indices M_2 , R_{-1} and *SCI*.

Theorem 3.3. *If G is a simple connected graph with $m \geq 1$ edges then*

$$ISI \leq \frac{(\Delta_e + \delta_e)(SCI)^2 R_{-1} M_2 - m^4}{\Delta_e \delta_e (SCI)^2 R_{-1}}. \tag{12}$$

Equality holds if and only if G is regular or semiregular bipartite graph.

Proof. For $r = 1$, $a_k := \sqrt{d_i + d_j}$, $b_k := \frac{1}{d_i d_j}$, where summation is performed over all edges in G , the inequality (2) transforms into

$$\sum_{i \sim j} d_i d_j (d_i + d_j) = \sum_{i \sim j} \frac{(\sqrt{d_i + d_j})^2}{\frac{1}{d_i d_j}} \geq \frac{\left(\sum_{i \sim j} \sqrt{d_i + d_j}\right)^2}{\sum_{i \sim j} \frac{1}{d_i d_j}},$$

i.e.

$$\sum_{i \sim j} d_i d_j (d_i + d_j) \geq \frac{\left(\sum_{i \sim j} \sqrt{d_i + d_j}\right)^2}{R_{-1}}. \tag{13}$$

By the arithmetic-harmonic mean inequality for real numbers (see e.g. [25]), we have

$$\left(\sum_{i \sim j} \sqrt{d_i + d_j}\right) \left(\sum_{i \sim j} \frac{1}{\sqrt{d_i + d_j}}\right) \geq m^2,$$

i.e.

$$\left(\sum_{i \sim j} \sqrt{d_i + d_j}\right)^2 \geq \frac{m^4}{(SCI)^2}. \tag{14}$$

Now, from (13) and (14), it follows that

$$\sum_{i \sim j} d_i d_j (d_i + d_j) \geq \frac{m^4}{(SCI)^2 R_{-1}}. \tag{15}$$

Eventually, the inequality (12) is obtained from (4) and (15).

Equality in (13) holds if and only if $d_i d_j (d_i + d_j) = c$, $c = \text{constant}$, for every edge in the graph G . Equality in (14) holds if and only if $d_i + d_j = c_1$, $c_1 = \text{constant}$, for every edge of G . Therefore, equality in (14) holds if and only if G is regular or semiregular bipartite graph. Consequently, it can be easily observed that equality in (12) holds if and only if G is regular or semiregular bipartite graph. \square

Corollary 3.3. *Let G be a simple connected graph with $m \geq 1$ edges. Then*

$$ISI \leq \frac{(\Delta_e + \delta_e)^2 (SCI)^2 R_{-1} M_2^2}{4\Delta_e \delta_e m^4}.$$

Equality holds if and only if G is regular or semiregular bipartite graph.

Next, we derive an upper bound on the ISI index in terms of graph parameters m, Δ_e, δ_e and topological indices M_2, Π_2, Π_1^* .

Theorem 3.4. *If G is a simple connected graph with $m \geq 1$ edges then*

$$ISI \leq \frac{(\Delta_e + \delta_e)M_2 - m (\Pi_1^*)^{\frac{1}{m}} (\Pi_2)^{\frac{1}{m}}}{\Delta_e \delta_e}, \tag{16}$$

with equality if and only if G is regular or semiregular bipartite graph.

Proof. Using the arithmetic-geometric mean inequality for real numbers (see e.g. [25]), we have

$$\sum_{i \sim j} d_i d_j (d_i + d_j) \geq m \left(\prod_{i \sim j} d_i d_j (d_i + d_j) \right)^{\frac{1}{m}} = m (\Pi_2)^{\frac{1}{m}} (\Pi_1^*)^{\frac{1}{m}}. \tag{17}$$

From (17) and (4), we obtain (16).

The equality sign holds throughout in (17) if and only if $d_i d_j (d_i + d_j) = c, c = \text{constant}$, for every edge of G . Therefore, equality in (17), and hence in (16), is attained if and only if G is regular or semiregular bipartite graph. \square

Corollary 3.4. *If G be a simple connected graph with $m \geq 1$ edges then*

$$ISI \leq \frac{1}{\Delta_e \delta_e} \left((\Delta_e + \delta_e)M_2 - \frac{m^2}{n} (\Pi_1^*)^{\frac{2}{m}} \right). \tag{18}$$

Equality holds if and only if G is regular or semiregular bipartite graph.

Proof. Since

$$n = \sum_{i \sim j} \left(\frac{1}{d_i} + \frac{1}{d_j} \right) = \sum_{i \sim j} \frac{d_i + d_j}{d_i d_j} \geq m \left(\prod_{i \sim j} \frac{d_i + d_j}{d_i d_j} \right)^{\frac{1}{m}} = m \frac{(\Pi_1^*)^{\frac{1}{m}}}{(\Pi_2)^{\frac{1}{m}}},$$

it follows

$$(\Pi_2)^{\frac{1}{m}} \geq \frac{m}{n} (\Pi_1^*)^{\frac{1}{m}}. \tag{19}$$

From (16) and (19), the required inequality (18) follows. \square

4. The best possible upper bound on the *ISI* index for binary trees

Sedlar *et al.* [31] derived the best possible upper bounds on the invariant *ISI* for several graph families. In [31], finding best possible upper bound on the aforementioned invariant for molecular trees (graphs representing alkanes) was left as an open problem. In this section, we will see that this problem can be easily solved for the case of binary trees [1] (that is, the trees with maximum degree at most 3). Binary trees actually form a subclass of the class of all molecular trees.

Because there is only one n -vertex tree for $n \leq 3$, so the problem of finding a bound on any topological index for trees make sense if $n \geq 4$.

Proposition 4.1. *For $n \geq 4$, if T is an n -vertex binary tree then*

$$ISI(T) \leq \begin{cases} \frac{9}{8}n - \frac{9}{4} & \text{if } n \text{ is even,} \\ \frac{9}{8}n - \frac{271}{120} & \text{otherwise,} \end{cases}$$

where the equality sign in the first inequality holds if and only if T contains no vertex of degree 2, and the equality sign in the second inequality holds if and only if T contains exactly one vertex of degree 2, which is adjacent to a pendant vertex and a vertex of degree 3.

Proof. Let $x_{i,j}$ be the number of edges in T connecting the vertices of degrees i and j . The invariant *ISI* of T can be calculated using the following formula.

$$ISI(T) = \frac{2}{3}x_{1,2} + \frac{3}{4}x_{1,3} + x_{2,2} + \frac{6}{5}x_{2,3} + \frac{3}{2}x_{3,3}. \tag{20}$$

If n_i is the number of vertices of degree i in the tree T then the following system of equations holds

$$n_1 + n_2 + n_3 = n, \tag{21}$$

$$n_1 + 2n_2 + 3n_3 = 2(n - 1), \tag{22}$$

$$x_{1,2} + x_{1,3} = n_1, \tag{23}$$

$$x_{1,2} + 2x_{2,2} + x_{2,3} = 2n_2, \tag{24}$$

$$x_{1,3} + x_{2,3} + 2x_{3,3} = 3n_3. \tag{25}$$

We solve the system of Equations (21)-(25) for the unknowns $n_1, n_2, n_3, x_{1,3}, x_{3,3}$. The values of $x_{1,3}$ and $x_{3,3}$ are given [1] below:

$$x_{1,3} = \frac{1}{4}(2n + 4 - 5x_{1,2} - 2x_{2,2} - x_{2,3}),$$

$$x_{3,3} = \frac{1}{4}(2n - 8 + x_{1,2} - 2x_{2,2} - 3x_{2,3}).$$

After substituting the values of $x_{1,3}$ and $x_{3,3}$ in Equation (20), we get:

$$ISI(T) = \frac{9}{8}n - \frac{9}{4} + \frac{5}{48}x_{1,2} - \frac{1}{8}x_{2,2} - \frac{9}{80}x_{2,3}. \tag{26}$$

Due to the constraint $n \geq 4$, it holds that $x_{1,2} \leq x_{2,2} + x_{2,3}$ and hence Equation (26) yields

$$ISI(T) \leq \frac{9}{8}n - \frac{9}{4} - \frac{1}{120}x_{2,3} - \frac{1}{48}x_{2,2}. \quad (27)$$

From Eqs. (21) and (22), it follows that

$$n - n_2 = 2(n_3 + 1),$$

which means that both the numbers n, n_2 are either even or odd. Now, (27) gives

$$ISI(T) \leq \begin{cases} \frac{9}{8}n - \frac{9}{4} & \text{if } n \text{ is even,} \\ \frac{9}{8}n - \frac{271}{120} & \text{if } n \text{ is odd,} \end{cases}$$

where the equality sign in the first inequality holds if and only if $x_{2,2} = x_{2,3} = 0$ (and hence $x_{1,2} = 0$), and the equality sign in the second inequality holds if and only if $x_{2,2} = 0, x_{2,3} = 1$ (and hence $x_{1,2} = 1$). \square

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