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Research Paper

New Results on Second Inverse Sum Indeg Index

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Abstract

The second inverse sum indeg topological index (ISI_2) is considered as a valuable tool for the study of graphs and trees. This index is systematically investigated for the first time, and its upper and lower bounds are derived for general graphs and trees. Furthermore, comparisons between ISI_2 and other existing topological indices are presented. The results demonstrate that ISI_2 not only provides valuable insights into the structure of graphs but also serves as a powerful instrument for modeling and analyzing complex networks, particularly in chemistry and pharmacology. Specifically, ISI_2 exhibits significant potential in predicting physicochemical properties of molecules, such as polarity, boiling point, and biological activity. Thus, ISI_2 may serve for the design and optimization of novel drug molecules and chemical compounds.

1 Introduction

Let G be an undirected graph, with the vertex and edge sets $V(G)$ and $E(G)$, respectively. Also, let $n = |V(G)|$ and $m = |E(G)|$ be the order and size of G. A topological index of the graph G is a numerical quantity related to G, reflecting some of its structural features. Some topological indices are important for their applications to various areas of knowledge, especially to chemistry [1]. Concerning their mathematical studies see, for instance, ([2–6]).

Several topological indices have been defined to describe molecules. One of the most important families of topological indices are the indices defined according to the distance of vertices in graphs. In the following, we introduce some of these indicators.

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The vertex PI index is defined as [7]:

$$PI_u(G) = \sum_{uv \in E(G)} (n_u + n_v),$$

where for an edge uv, n_u is the number of vertices of graph G lying closer to u than v, and n_v is the number of vertices of graph G lying closer to v.

The PI topological index is a useful tool in computational chemistry that helps in better understanding molecular structures and predicting their properties [8–10]. The vertex Szeged index is another topological index, defined as [11]:

$$Sz\,(G) = \sum_{uv \in E(G)} n_u\, n_v.$$

The Szeged topological index is used to predict physical and chemical properties of molecules, such as boiling point, stability of molecules, and other properties. This index is especially popular in quantum chemistry due to its simplicity and efficiency [12].

The second geometric-arithmetic index is defined as [13]:

$$GA_2\,(G) = \sum_{uv \in E(G)} \frac{2\sqrt{n_u n_v}}{n_u + n_v}.$$

The lower and upper bounds on the second geometric-arithmetic index (GA_2) and the characterization of the extremal graphs are reported in [14]. In [15], the trees with second minimum and maximum GA_2 are characterized, as well as the unicyclic graphs with minimum and maximum GA_2. A new study on trees and unicyclic graphs was done in [16].

Graovac and Ghorbani in [17] defined the second atom–bond connectivity index as follows:

$$ABC_2\,(G) = \sum_{uv \in E(G)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}}.$$

The new lower and upper bounds for the $ABC_2(G)$ in graphs and trees are determined in [18]. Further studies on the second atom–bond connectivity index were conducted by Rostami et al. in [19]. The relations between the second geometric-arithmetic index and the second atom-bond connectivity index for the general and special class of graphs has been obtained in [20].

The second inverse sum indeg (henceforth, ISI_2) index of a graph G is defined as [21]:

$$ISI_2\,(G) = \sum_{uv \in E(G)} \frac{n_u n_v}{n_u + n_v}.$$

In this paper, we establish new bounds on the ISI_2 index using other graph invariants, and determine the trees with the minimum and maximum ISI_2 index.

2 Lower and upper bounds for the ISI_2

Let K_n, C_n, S_n and P_n, be the complete graph, cycle, star, and path on n vertices, respectively. Let $K_{n,m}$ be the complete bipartite graph on n and m vertices in its two partition sets, respectively.

We call a graph $G = (V, E)$ distance-balanced if with $n_u = n_v$ for each edge $uv \in E$. In this section, we give some basic mathematical features of the second inverse sum indeg.

Example 2.1. Let n be a natural number. Then, by using a simple calculation, one can show that

(i) $ISI_2(C_n) = \begin{cases} \frac{n(n-1)}{4}, & \text{if } n \text{ is odd}, \\ \frac{n^2}{4}, & \text{if } n \text{ is even}. \end{cases}$

(ii) $ISI_2(K_n) = \frac{n(n-1)}{4}$,

(iii) $ISI_2(K_{n,m}) = \frac{(nm)^2}{n+m}$.

In the next theorem, we determine lower and upper bounds for ISI_2 for a connected graph with n vertices and m edges.

Theorem 2.2. *Let G be a graph with n vertices and m edges. Then*

$$\frac{m}{n} \leq ISI_2(G) \leq \frac{mn^2}{8}.$$

Equality holds if and only if graph $G \cong K_2$.

Proof. For all edges uv we know that $n_u \geq 1$, $n_v \geq 1$ and $n_u + n_v \leq n$, thus $n_u + n_v \geqslant 2$ so

$$n_u + n_v \leqslant \frac{1}{2}, \tag{1}$$

and $n_u + n_v \leqslant n$, thus

$$n_u n_v \leqslant \frac{n^2}{4}. \tag{2}$$

Hence, (1) and (2) inclouded

$$\frac{n_u n_v}{n_u + n_v} \leqslant \frac{n^2}{8},$$

and finally

$$ISI_2(G) = \sum_{uv \in E(G)} \frac{n_u n_v}{n_u + n_v} \leqslant \frac{mn^2}{8}.$$

Now, Let $uv \in E(G)$ be an arbitrary edge in G. Then we have $n_u, n_v \geq 1$, so $n_u n_v \geq 1$. Also $n_u + n_v \leq n$ and $\frac{1}{n_u+n_v} \geq \frac{1}{n}$, therefore

$$ISI_2(G) = \sum_{uv \in E(G)} \frac{n_u n_v}{n_u + n_v} \geq \sum_{uv \in E(G)} \frac{1}{n} = \frac{m}{n}.$$

Equality in (1) occurs if and only if $n_u = n_v = 1$ holds for all edge uv and equality in (2) occurs if and only if $n = 2$ which implies $G \cong K_2$. ∎

Example 2.3. Let n and i be natural numbers such that $i < n$ and $G \cong C_n$ when n is an even, $G \cong K_{i,n-i}$ or $G \cong T_n$. Then

$$ISI_2(G) = \frac{Sz_u(G)}{n}.$$

Theorem 2.4. *Let G be a complete bipartite graph with $n \geq 4$ vertices. Then*

$$\frac{(n-1)^2}{n} \leq ISI_2(G) \leq f(n),$$

in which

$$f(n) = \begin{cases} \frac{n^3}{16}, & if\, n\, is\, even, \\ \frac{(n^2-1)^2}{16n}, & if\, n\, is\, odd, \end{cases}$$

the lower bound occurs for the $K_{1,n-1}$ and the upper bound occurs for the $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

Proof. If G is a connected complete bipartite graph with n vertices, then for any edge uv of graph G we have $n_u + n_v = n$. So

$$ISI_2(G) = \frac{1}{n} \sum_{uv \in E(G)} n_u n_v.$$

Suppose the vertices set of graph G partitioned into two sets V_1 and V_2. We assume $|V_1| = v$ and $|V_2| = n - v$ and it is clear that $|V_1| + |V_2| = n$. The number of edges in graph G is $v(n-v)$, and for any edge uv of graph G we have $n_u = v$ and $n_v = n - v$ where $1 \leq v \leq n-1$. Then, the second inverse sum indeg index of complete bipartite graph with $n \geq 4$ vertices as follows:

$$ISI_2(G) = \frac{v^2(n-v)^2}{n} = g(v).$$

By simple calculation in function $g(v)$ we can show that the maximum and minimum values of $g(v)$ happen if $v = \frac{n}{2}$ for n is even or $v = \frac{n-1}{2}$ for n is odd and $v = 1$ respectively. So

$$g(\frac{n}{2}) = \frac{n^3}{16},$$

or

$$g(\frac{n-1}{2}) = \frac{(n^2-1)^2}{16n},$$

and

$$g(1) = \frac{(n-1)^2}{n}.$$

It is clear that the lower bound occurs for the $K_{1,n-1}$ and the upper bound occurs for the $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$. ■

Theorem 2.5. *Let T be a tree with n vertices. Then*

$$\frac{(n-1)^2}{n} \leq ISI_2(T) \leq \frac{n(n-1)}{4},$$

the lower bound occurs for the S_n and the upper bound occurs for P_2.

Proof. For any edge uv of trees T we have $n_u + n_v = n$, then $ISI_2(T)$ is simplified as:

$$ISI_2(T) = \sum_{uv \in E(G)} \frac{n_u n_v}{n_u + n_v} = \frac{1}{n} \sum_{uv \in E(G)} n_u n_v.$$

On the other hand, it is clear that the summation on the right-hand side of the above formula goes over $n-1$ terms. The equality $n_u + n_v = n$ implies that the minimum and maximum value of $n_u n_v$ are $n-1$ and $\frac{n^2}{4}$, therefore $n-1 \leq n_u n_v \leq \frac{n^2}{4}$. Hence, $\frac{n-1}{n} \leq \frac{n_u n_v}{n} \leq \frac{n}{4}$ and so

$$\sum_{uv\in E(T)} \frac{n-1}{n} \leq \sum_{uv\in E(T)} \frac{n_u n_v}{n} \leq \sum_{uv\in E(T)} \frac{n}{4}.$$

This means that

$$\frac{(n-1)^2}{n} \leq ISI_2\,(T) \leq \frac{n\,(n-1)}{4}.$$

Note that equality occurs if and only if $n_u = 1$ and $n_v = n-1$ holds for all $e = uv \in E(T)$, which implies the only such tree is star. The upper bound is attained when, for every edge in the tree T, we have $n_u = n_v = \frac{n}{2}$, a condition that is exclusively satisfied by the P_2 tree. Hence, the proof is complete. ∎

To determine the tree with the maximum ISI_2-value, we first establish an auxiliary result. Consider the trees T_1 and T_2 with n-vertex illustrated in Figure 1. These two trees differ only in the position of a terminal vertex. In tree T_2 the terminal vertex is moved from the b-branch to the a-branch. Hereafter, we assume that $a \geq b$. The difference in the ISI_2-values of T_1 and T_2, is examined in the following expression:

$$ISI_2\,(T_1) - ISI_2\,(T_2) = \frac{1}{n}\left(\sum_{uv\in E(T_1)} n_u n_v - \sum_{u'v'\in E(T_1)} n_{u'} n_{v'}\right).$$

All terms cancel out except the terms pertaining to the edges indicated by arrows in Figure 1, in which, for edge $e = uv$ of tree T_1 we have $n_u n_v = b(n-b)$ and for edge $e = u'v'$ of tree T_2 we have $n'_u n'_v = (a+1)(n-a-1)$. Using

$$b(n-b) - (a+1)(n-a-1) = (a-b+1)(a+b+1-n),$$

we have

$$ISI_2\,(T_1) - ISI_2\,(T_2) = \frac{1}{n}\,(a-b+1)\,(a+b+1-n)\,.$$

Based on the above formula, we know that, $a-b+1 \geq 0$ and $a+b+1-n \leq 0$. Thus

$$ISI_2\,(T_1) - ISI_2\,(T_2) \leq 0.$$

In other words, the conversion $T_1 \to T_2$, wherein a node from a shorter branch is relocated to a longer branch, increases the second inverse sum indeg index. We are now prepared to present and demonstrate the following theorem.

Theorem 2.6. *The path P_n is the n-vertex tree with the maximum second inverse sum indeg index and its value is equal to:*

$$ISI_2\,(P_n) = \frac{n^2-1}{6}.$$

Proof. By continuing the described transformation $T_1 \to T_2$, we can move all vertices from the shorter branch to the longer branch, while the value of ISI_2 keeps increasing. By repeatedly applying this transformation sufficiently many times, we will ultimately arrive at the path P_n. The value of the second inverse sum indeg index for the path P_n is equal to:

$$ISI_2\,(P_n) = \frac{1}{n}\sum_{uv\in E(P_n)} n_u n_v = \frac{1}{n}\sum_{i=1}^{n-1} i\,(n-i) = \frac{n^2-1}{6}.$$

This complete the proof. ∎

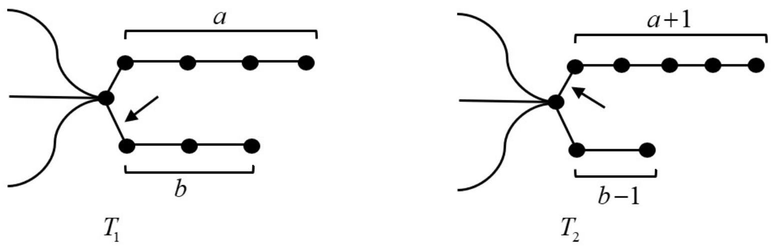

Figure 1: The transformation $T_1 \to T_2$ increases the ISI_2 index provided $a \geq b$.

3 Relationships between ISI_2 and other topological indices

In this section, we present some new results relating between some familiar topological indices, including the second atom bond connectivity index, the second geometric-arithmetic index, the vertex PI index, and the inverse sum indeg index ISI_2.

Theorem 3.1. *Let G be a graph with n vertices and m edges. Then*

$$\frac{Sz_u(G)}{n} \leq ISI_2(G) \leq \frac{1}{2} Sz_u(G).$$

Equality in the lower bound holds if and only if $n_u + n_v = n$ holds for all edge uv. Moreover, equality in the upper bound holds if and only if G is a complete graph.

Proof. For all edges uv, we know that $n_u \geq 1$, $n_v \geq 1$, then $n_u + n_v \geqslant 2$, thus

$$\frac{1}{n_u + n_v} \leqslant \frac{1}{2}.$$

So

$$ISI_2(G) = \sum_{uv \in E(G)} \frac{n_u n_v}{n_u + n_v} \leq \frac{1}{2} \sum_{uv \in E(G)} n_u n_v = \frac{1}{2} Sz(G).$$

The above equality occurs if and only if $n_u = n_v = 1$ holds for all edge uv, which implies $G \cong K_n$.

Now, let $uv \in E(G)$ be an arbitrary edge in G. Then we have $n_u + n_v \leq n$ and $\frac{1}{n_u+n_v} \geq \frac{1}{n}$, so

$$ISI_2(G) = \sum_{uv \in E(G)} \frac{n_u n_v}{n_u + n_v} \geq \sum_{uv \in E(G)} \frac{n_u n_v}{n} = \frac{Sz_u(G)}{n}.$$

The above equality occurs if and only if $n_u + n_v = n$ holds for all edge uv. ■

In the following theorem, we establish relationships between topological indices ISI_2, ABC_2, GA_2, and Sz_u.

Theorem 3.2. *Let G be the arbitrary distance-balanced graph of order n with m edges, such that $n_u = n_v = \delta$. Then*

(i) if $\delta = 1$, then

$$ABC_2(G) < ISI_2(G) < GA_2(G) = Sz_u(G) < PI_u(G).$$

(ii) If $\delta = 2$*, then*

$$ABC_2(G) < GA_2(G) = ISI_2(G) < PI_u(G) = Sz_u(G).$$

(iii) If $\delta \geq 3$*, then*

$$ABC_2(G) < GA_2(G) < ISI_2(G) < PI_u(G) < Sz_u(G).$$

Proof. Assume $n_u = n_v = \delta$ for each edge uv of a distance-balanced graph G. Then

$$\begin{array}{l} PI_u(G) = 2m\delta, \\ Sz_u(G) = m\delta^2, \\ GA_2(G) = m, \\ ABC_2(G) = \frac{m\sqrt{2\delta-2}}{\delta}, \\ ISI_2(G) = \frac{m\delta}{2}. \end{array}$$

Now, for $\delta = 1$ we have,

$$\begin{array}{l} ABC_2(G) = 0, \\ ISI_2(G) = \frac{m}{2}, \\ GA_2(G) = m, \\ Sz_u(G) = m, \\ PI_u(G) = 2m. \end{array}$$

Since the value of m is a natural number greater than or equal to one, so (i) holds.

Similarly, for $\delta = 2$ we have,

$$\begin{array}{l} ABC_2(G) = \frac{m\sqrt{2}}{2}, \\ GA_2(G) = m, \\ ISI_2(G) = m, \\ PI_u(G) = 4m, \\ Sz_u(G) = 4m. \end{array}$$

Thus (ii) holds.

Finally, for $\delta \geq 3$ according to Theorem 3.1 in [20], and with simple calculations it can be shown that

$$ABC_2(G) < GA_2(G) < ISI_2(G) < PI_u(G) < Sz_u(G).$$

Thus, the proof is complete. ■

Corollary 3.3. *The following assertions hold:*

(i) $ABC_2(K_n) < ISI_2(K_n) < GA_2(K_n) = Sz_u(K_n) < PI_u(K_n)$.

(ii) If $n \geq 3$*, then*

$$ABC_2(K_{n,n}) < GA_2(K_{n,n}) < ISI_2(K_{n,n}) < PI_u(K_{n,n}) < Sz_u(K_{n,n}).$$

(iii) If $n \in \{4, 5\}$*, then*

$$ABC_2(C_n) < GA_2(C_n) = ISI_2(C_n) < PI_u(C_n) = Sz_u(C_n),$$

and if $n \geq 6$*, then*

$$ABC_2(C_n) < GA_2(C_n) < ISI_2(C_n) < PI_u(C_n) < Sz_u(C_n).$$

Proof. (i) We consider the complete graph K_n. For each edge uv we have $n_u = n_v = 1$, then by Theorem 3.2, we conclude

$$ABC_2(K_n) < ISI_2(K_n) < GA_2(K_n) = Sz_u(K_n) < PI_u(K_n).$$

(ii) We evaluate the result for the complete bipartite graph $K_{n,n}$. Since $K_{1,1} \cong K_2$ and $K_{2,2} \cong C_4$ so, it is sufficient to continue the investigation for $n \geq 3$. Hence, for each edge of $K_{n,n}$ we have $n_u = n_v = n$, thus

$$ABC_2(K_{n,n}) < GA_2(K_{n,n}) < ISI_2(K_{n,n}) < PI_u(K_{n,n}) < Sz_u(K_{n,n}).$$

(iii) Now we consider cycle graph C_n for each edge uv, it is clear that $n_u = n_v = \frac{n}{2}$ if n is even and $n_u = n_v = \frac{n-1}{2}$ if n is odd, then by Theorem 3.2 for $n \in \{4, 5\}$

$$ABC_2(C_n) < GA_2(C_n) = ISI_2(C_n) < PI_u(C_n) = Sz_u(C_n),$$

and for $n \geq 6$,

$$ABC_2(C_n) < GA_2(C_n) < ISI_2(C_n) < PI_u(C_n) < Sz_u(C_n).$$

Thus, the corollary is proved. ∎

We will require the following two lemmas, which we state below.

Lemma 3.4. *Let $a = \{a_i\}_{i=1}^n$ and $b = \{b_i\}_{i=1}^n$ be two sequences of positive numbers. Then,*

$$\sum_{i=1}^{n} \frac{a_i}{b_i} \geq \frac{\sum_{i=1}^{n} a_i}{\sum_{i=1}^{n} b_i},$$

with equality if $n = 1$.

Proof. Let $B = \prod_{i=1}^{n} b_i$ and $\frac{B}{b_j} = B_j = \prod_{\substack{i=1 \\ i \neq j}}^{n} b_i$. Then

$$\begin{aligned}
\left(\sum_{i=1}^{n} b_i\right)\left(\sum_{i=1}^{n} B_i a_i\right) &= \sum_{j=1}^{n}\sum_{i=1}^{n} b_j B_i a_i \\
&= \sum_{j=1}^{n}\sum_{\substack{i=1 \\ i \neq j}}^{n} b_j B_i a_i + \sum_{i=1}^{n} b_i B_i a_i \\
&= \sum_{j=1}^{n}\sum_{\substack{i=1 \\ i \neq j}}^{n} b_j B_i a_i + B\sum_{i=1}^{n} a_i \\
&\geq B\sum_{i=1}^{n} a_i.
\end{aligned}$$

Therefore,

$$\frac{\left(\sum_{i=1}^{n} b_i\right)\left(\sum_{i=1}^{n} B_i a_i\right)}{\sum_{i=1}^{n} b_i} \geq B\frac{\sum_{i=1}^{n} a_i}{\sum_{i=1}^{n} b_i},$$

and finally

$$\sum_{i=1}^{n} \frac{a_i}{b_i} = \sum_{i=1}^{n} \frac{B_i a_i}{B} \geq \frac{\sum\limits_{i=1}^{n} a_i}{\sum\limits_{i=1}^{n} b_i},$$

and the proof is complete. It is very clear that equality holds for $n = 1$. ■

Lemma 3.5. *Let $a = \{a_i\}_{i=1}^{n}$ and $b = \{b_i\}_{i=1}^{n}$ be two sequences of positive numbers. Then,*

$$\sum_{i=1}^{n} a_i b_i \leq \left(\sum_{i=1}^{n} a_i\right)\left(\sum_{i=1}^{n} b_i\right),$$

with equality if $n = 1$.

Proof. The proof is clear. ■

In the following, we prove inequalities that demonstrate the relationship between the Szeged topological index, the vertex PI index, and the inverse sum indeg index ISI_2.

Theorem 3.6. *Let G be a graph on n vertices and m edges. Then*

$$ISI_2(G) \geq \frac{Sz_u(G)}{PI_u(G)},$$

with equality if and only if graph $G \cong K_2$.

Proof. For all edges uv we know that $n_u \geq 1$, $n_v \geq 1$, then $n_u n_v \geq 1$ and $n_u + n_v \geq 2$. Therefore by Lemma 3.4

$$ISI_2(G) = \sum_{uv \in E(G)} \frac{n_u n_v}{n_u + n_v} \geq \frac{\sum\limits_{uv \in E(G)} n_u n_v}{\sum\limits_{uv \in E(G)} n_u + n_v} = \frac{Sz_u(G)}{PI_u(G)}.$$

The above inequality holds when the graph has only one edge, and this only happens for K_2. ■

Theorem 3.7. *Let G be a graph with n vertices and m edges. Then*

$$ISI_2(G) \geq \frac{m^2}{PI_u(G)},$$

with equality if and only if graph $G \cong K_2$.

Proof. For all edges uv we know that $n_u \geq 1$, $n_v \geq 1$, then $n_u n_v \geq 1$. Thus

$$ISI_2(G) = \sum_{uv \in E(G)} \frac{n_u n_v}{n_u + n_v} \geq \sum_{uv \in E(G)} \frac{1}{n_u + n_v}.$$

Now, by applying the Cauchy–Schwarz inequality, we know that $\sum\limits_{i=1}^{n} \frac{1}{b_i} \geq \frac{n^2}{\sum\limits_{i=1}^{n} b_i}$. So,

$$ISI_2(G) \geq \sum_{uv \in E(G)} \frac{1}{n_u + n_v} \geq \frac{m^2}{\sum\limits_{uv \in E(G)} n_u + n_v} = \frac{m^2}{PI_u(G)}.$$

The above inequality holds when we have for the graph $n_u = n_v = 1$ and $n_u + n_v$ is a constant, which happens for the complete graph K_n. ■

Theorem 3.8. *Let G be a graph on n vertices and m edges. Then*

$$ISI_2(G) \leq \frac{PI_u(G)}{4},$$

with equality if and only if graph G is distance-balanced.

Proof. Let $uv \in E(G)$ be an arbitrary edge in G (so that $n_u, n_v \neq 0$). From

$$0 \leq (n_u - n_v)^2,$$

we get, after adding $4n_u n_v$ to both sides, that

$$4n_u n_v \leq (n_u + n_v)^2.$$

So that after division with $4(n_u + n_v)$, it follows that

$$\frac{n_u n_v}{n_u + n_v} \leq \frac{n_u + n_v}{4}.$$

Now, we have

$$ISI_2(G) = \sum_{uv \in E(G)} \frac{n_u n_v}{n_u + n_v} \leq \sum_{uv \in E(G)} \frac{n_u + n_v}{4} = \frac{PI_u(G)}{4}.$$

Equality holds if and only if $n_u = n_v$ for each edge $uv \in E(G)$, then distance-balanced graph G. ■

Theorem 3.9. *Let G be a graph on n vertices and m edges. Then*

$$ISI_2(G) \leq \frac{1}{2}\left(PI_u(G) - m\right),$$

with equality if and only if graph $G \cong K_n$.

Proof. According to the definition of the second inverse sum indeg index, we have

$$\begin{aligned}
2ISI_2(G) + m &= \sum_{uv \in E(G)} \frac{2n_u n_v}{n_u + n_v} + \sum_{uv \in E(G)} 1 = \sum_{uv \in E(G)} \left(\frac{2n_u n_v}{n_u + n_v} + 1\right) \\
&= \sum_{uv \in E(G)} \left(\frac{n_u + n_v + 2n_u n_v}{n_u + n_v}\right) \\
&\leq \sum_{uv \in E(G)} \left(\frac{{n_u}^2 + {n_v}^2 + 2n_u n_v}{n_u + n_v}\right) \\
&= \sum_{uv \in E(G)} \frac{(n_u + n_v)^2}{n_u + n_v} = PI_u(G).
\end{aligned}$$

Therefore,

$$ISI_2(G) \leq \frac{1}{2}\left(PI_u(G) - m\right).$$

The above equality holds if and only if $n_u = n_v = 1$ for each edge $uv \in E(G)$, then $G \cong K_n$. ■

Theorem 3.10. *Let G be a graph on n vertices and m edges. Then*

$$ISI_2(G) \leq \frac{1}{4}(PI_u(G))(Sz_u(G)).$$

with equality if and only if graph $G \cong K_n$.

Proof. For all edges uv we know that $n_u \geq 1$, $n_v \geq 1$, then $n_u + n_v \geq 2$, so $(n_u + n_v)^2 \geq 4$. Thus

$$\frac{1}{(n_u + n_v)^2} \leq \frac{1}{4},$$

hence,

$$\frac{1}{(n_u + n_v)} \leq \frac{(n_u + n_v)}{4},$$

therefore,

$$\frac{n_u n_v}{n_u + n_v} \leq \frac{1}{4}(n_u n_v)(n_u + n_v).$$

By summing the sides of the above inequality over all edges of the graph G, we have

$$ISI_2(G) = \sum_{uv \in E(G)} \frac{n_u n_v}{n_u + n_v} \leq \frac{1}{4} \sum_{uv \in E(G)} (n_u n_v)(n_u + n_v).$$

Now, by Lemma 3.5, we can write

$$ISI_2(G) \leq \frac{1}{4} \sum_{uv \in E(G)} (n_u n_v) \sum_{uv \in E(G)} (n_u + n_v) = \frac{1}{4} Sz_u(G)\, PI_u(G).$$

Hence, the proof is complete. ■

The sigma index of G is defined in [22] as:

$$\sigma(G) = \sum_{uv \in E(G)} (d_u - d_v)^2,$$

where, d_u is the degree of u.

It seems quite natural to define the second sigma index of G as follows:

$$\sigma_2(G) = \sum_{uv \in E(G)} (n_u - n_v)^2.$$

Theorem 3.11. *Let G be a graph on n vertices and m edges. Then*

$$ISI_2(G) \leq \frac{1}{4}\left(PI_u(G) - \frac{\sigma_2(G)}{n}\right).$$

Equality occurs when for each edge we have $n_u + n_v = n$.

Proof. For two real numbers a and b, we have that

$$ab = \frac{1}{4}\left((a+b)^2 - (a-b)^2\right),$$

so,

$$n_u n_v = \frac{1}{4}\left[(n_u + n_v)^2 - (n_u - n_v)^2\right].$$

Therefore,

$$\frac{n_u n_v}{n_u + n_v} = \frac{1}{4}\left[(n_u + n_v) - \frac{(n_u - n_v)^2}{n_u + n_v}\right].$$

On the other hand, $n_u + n_v \leq n$ and $-\frac{1}{n_u+n_v} \leq -\frac{1}{n}$, and finally

$$ISI_2(G) \leq \frac{1}{4}\left(PI_u(G) - \frac{\sigma_2(G)}{n}\right).$$

It is simply clear that the above equality holds if and only if $n_u + n_v = n$ for each edge $uv \in E(G)$. For example, for cycle graph when the number of vertices is an even. Also for a complete bipartite graph or tree graph with n vertices. ■

Theorem 3.12. *Let G be a graph on n vertices and m edges. Then*

$$ISI_2(G) \geq 2m - PI_u(G).$$

Equality occurs when for each edge we have $n_u = n_v = 1$.

Proof. From the fact that $a + \frac{1}{a} \geq 2$ for any real number $a > 0$, we have

$$ISI_2(G) + PI_u(G) = \sum_{uv\in E(G)} \frac{n_u n_v}{n_u + n_v} + \sum_{uv\in E(G)} n_u + n_v.$$

On the other hand, $n_u n_v \geq 1$ and $\frac{1}{n_u n_v} \leq 1$, so

$$\begin{aligned} \sum_{uv\in E(G)} \frac{n_u n_v}{n_u + n_v} + \sum_{uv\in E(G)} n_u + n_v &\geq \sum_{uv\in E(G)} \frac{n_u n_v}{n_u + n_v} + \sum_{uv\in E(G)} \frac{n_u + n_v}{n_u n_v} \\ &= \sum_{uv\in E(G)} \left(\frac{n_u n_v}{n_u + n_v} + \frac{n_u + n_v}{n_u n_v}\right) \\ &\geq 2m. \end{aligned}$$

Therefore, $ISI_2(G) \geq 2m - PI_u(G)$. Above equality holds if and only if $n_u = n_v = 1$ for each edge $uv \in E(G)$, then $G \cong K_n$. ■

In the next, we prove inequalities that demonstrate the relationship between ABC_2, and ISI_2. First, we prove the following lemma.

Lemma 3.13. *Let $f(x,y) = x^3y^3 - x^3 - y^3 - 3x^2y - 3xy^2 + 2x^2 + 2y^2 + 4xy$. Then for $2 \leq x \leq y$ we have $f(x,y) > 0$, and for $2 \leq x$ we have $f(x,1) < 0$.*

$$\begin{cases} f(x,y) > 0, & 2 \leq x \leq y, \\ f(x,1) < 0, & 2 \leq x, \\ f(1,1) > 0. & \end{cases}$$

Proof. For all $(x, y) \in R^2$ we have $f(x, y) = f(y, x)$, then the function f can be classified as follows:

$$\begin{aligned} f(x,y) &= x^3y^3 - x^3 - y^3 - 3x^2y - 3xy^2 + 2x^2 + 2y^2 + 4xy \\ &= 7\frac{x^3y^3}{4} - x^3 + \frac{x^3y^3}{4} - y^3 + \frac{x^3y^3}{4} - 3x^2y + \frac{x^3y^3}{4} - 3xy^2 + 2x^2 \\ &+ 2y^2 + 4xy \\ &= x^3\left(\frac{y^3}{4} - 1\right) + y^3\left(\frac{x^3}{4} - 1\right) + x^2y\left(\frac{xy^2}{4} - 3\right) + xy^2\left(\frac{x^2y}{4} - 3\right) \\ &+ 2x^2 + 2y^2 + 4xy, \end{aligned}$$

with a simple check, it can be shown that for $3 \leq x \leq y$ we have $f(x, y) \geq 0$. Continuing the proof of this lemma, we are reviewing $f(x, 2)$.

$$\begin{aligned} f(x,2) = 7x^3 - 4x^2 - 4x &= x\left(7x^2 - 4x - 4\right) \\ &= x\left(x^2 - 4x + 4 + 6x^2 - 8\right) \\ &= x\left((x-2)^2 + 6x^2 - 8\right) \geq 32. \end{aligned}$$

As a result, for $2 \leq x \leq y$ we have $f(x, y) > 0$.

Now, we investigate $f(x, 1)$,

$$f(x,1) = -x^2 + x + 1 = -(x - \frac{1}{2})^2 + \frac{5}{4}.$$

If $x \geq 2$, then $f(x, 1) \leq -1 < 0$. ■

Theorem 3.14. *Let G be a graph with $n \geq 3$ vertices. Then*

$$\begin{cases} ISI_2(G) > ABC_2(G), & G \ncong S_n, \\ ISI_2(G) < ABC_2(G), & G \cong S_n. \end{cases}$$

Proof. For any edge uv of graph G

$$\begin{aligned} \frac{n_u n_v}{n_u + n_v} &> \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} \\ &\Leftrightarrow \frac{(n_u n_v)^2}{(n_u + n_v)^2} > \frac{n_u + n_v - 2}{n_u n_v} \\ &\Leftrightarrow (n_u n_v)^3 > (n_u + n_v)^2 (n_u + n_v - 2) \\ &\Leftrightarrow (n_u n_v)^3 - (n_u)^3 - (n_v)^3 - 3(n_u)^2 n_v - 3n_u (n_v)^2 \\ &+ 2(n_u)^2 + 2(n_v)^2 + 4n_u n_v > 0. \end{aligned}$$

Now we consider

$$\begin{aligned} f(n_u, n_v) = (n_u n_v)^3 - (n_u)^3 - (n_v)^3 - 3(n_u)^2 n_v \\ -3n_u (n_v)^2 + 2(n_u)^2 + 2(n_v)^2 + 4n_u n_v. \end{aligned}$$

If $n_u = x$ and $n_v = y$, then by Lemma 3.13 we have $f(n_u, n_v) = f(x, y) > 0$, for $2 \leq x \leq y$. Therefore, if for every edge e in graph G, the $n_u, n_v \geq 2$, then the $ABC_2(G)$ is smaller than the $ISI_2(G)$. Furthermore, if for all edges $e = uv$ in graph G, exactly one of the n_u or n_v has equal to 1, then the $ABC_2(G)$ is greater than the $ISI_2(G)$. This condition holds exclusively for star graph S_n. ■

Theorem 3.15. *Let G be a graph on n vertices and m edges. Then*

$$\frac{1}{2} GA_2(G) \leq ISI_2(G),$$

with equality if and only if graph $G \cong K_n$.

Proof. For all edges uv we know that $n_u \geq 1$, $n_v \geq 1$, then $n_u n_v \geq 1$, and $\sqrt{n_u n_v} \leq n_u n_v$. So

$$\frac{\sqrt{n_u n_v}}{n_u + n_v} \leq \frac{n_u n_v}{n_u + n_v}.$$

By summing the sides of the above inequality over all edges of the graph G, we have

$$\frac{1}{2} GA_2(G) = \sum_{uv \in E(G)} \frac{\sqrt{n_u n_v}}{n_u + n_v} \leq \sum_{uv \in E(G)} \frac{n_u n_v}{n_u + n_v} = ISI_2(G).$$

The above equality holds if and only if $n_u = n_v = 1$ for each edge $uv \in E(G)$, then $G \cong K_n$. ■

4 Concluding remarks

In the present research, the topological index ISI_2 was considered as a valuable tool for the analysis of graphs and trees. The upper and lower bounds on this index were derived for general graphs and trees, providing a deeper understanding of its behavior in graph structures and laying the groundwork for future research in this area.

Another achievement of the present work is the comparison with other earlier established topological indices, revealing that ISI_2 offers complementary and sometimes unique insights into graph properties. Notably, the index exhibits distinct behavior in specific graph structures such as trees and star graphs, making it particularly useful in practical applications, including computational chemistry, network analysis, and drug molecule design.

Based on these findings, it is recommended that future studies explore the application of ISI_2 in molecular modeling, prediction of physicochemical properties, and optimization of molecular structures. Additionally, investigating the correlation of this index with other chemical and biological parameters could open new avenues in this field.

It is hoped that the results of this research will inspire further investigations and advancements in this area.

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