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Research article

On the variable inverse sum deg index

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Abstract: Several important topological indices studied in mathematical chemistry are expressed in the following way $\sum_{uv\in E(G)} F(d_u, d_v)$, where F is a two variable function that satisfies the condition $F(x, y) = F(y, x)$, uv denotes an edge of the graph G and d_u is the degree of the vertex u. Among them, the variable inverse sum deg index ISD_a, with $F(d_u, d_v) = 1/(d_u^a + d_v^a)$, was found to have several applications. In this paper, we solve some problems posed by Vukičević [1], and we characterize graphs with maximum and minimum values of the ISD_a index, for $a < 0$, in the following sets of graphs with n vertices: graphs with fixed minimum degree, connected graphs with fixed minimum degree, graphs with fixed maximum degree, and connected graphs with fixed maximum degree. Also, we performed a QSPR analysis to test the predictive power of this index for some physicochemical properties of polyaromatic hydrocarbons.

Keywords: variable inverse sum deg index; inverse sum indeg index; optimization on graphs; degree-based topological index

1. Introduction

Topological indices have become an important research topic associated with the study of their mathematical and computational properties and, fundamentally, for their multiple applications to various areas of knowledge (see, e.g., [2–9]). Within the study of mathematical properties, we will contribute to the study of the optimization problems involved with topological indices (see, e.g., [10–18]).

In [19, 20] several degree-based topological indices, called *adriatic indices*, were presented; one of them is the *inverse sum indeg* index *ISI*. It is important to note that this index was selected as one of the most predictive, in particular associated with the total surface area of the isomers of octane.

Let G be a graph and $E(G)$ the set of all edges in G, denote by uv the edge of the graph G with vertices u, v and d_z is the degree of the vertex z. the ISI index is defined by

$$ISI(G) = \sum_{uv\in E(G)} \frac{1}{\frac{1}{d_u} + \frac{1}{d_v}} = \sum_{uv\in E(G)} \frac{d_u\, d_v}{d_u + d_v} .$$

Nowadays, this index has become one of the most studied from the mathematical point of view (see, e.g., [21–27]). We study, here, the mathematical properties of the *variable inverse sum deg index* defined, for each $a \in \mathbb{R}$, as

$$ISD_a(G) = \sum_{uv\in E(G)} \frac{1}{d_u^a + d_v^a} .$$

Note that ISD_{-1} is the inverse sum indeg index ISI.

This research is motivated, in general, by the theoretical-mathematical importance of the topological indices and by their applicability in different areas of knowledge (see [28–30]). Additionally, in particular, by the work developed by Vukičević entitled "Bond Additive Modeling 5. Mathematical Properties of the Variable Sum Exdeg Index" (see [1]), where several open problems on the topological index ISD_a were proposed. The novelty of this work is given in two main directions. The first one is associated with the solution of some of the problems posed in [1]. The second one is associated with the development of new optimization techniques and procedures related to the monotony and differentiation of symmetric functions, which allowed us to solve extremal problems and to present bounds for ISD_a. Although, these techniques can be extended or applied in a natural way to obtain new relations and properties of other topological indices, it should be noted that their applicability requires the monotony of the function that determines the index to be studied.

In Section 2, we find optimal bounds and solve extremal problems associated with the topological index ISD_a, with $a < 0$, for several families of graphs. In Proposition 4, we solve the extremal problems for connected graphs with a given number of vertices. Theorem 6 and Remark 1 solve these problems for graphs with a given number of vertices and minimum degree; similarly, Theorems 8 and 9 present solutions to extremal problems in connected graphs with a given number of vertices and maximum degree. In this direction, in Theorem 5, Proposition 7 and Theorem 10, we present optimal bounds for the studied index.

In Section 3 of this research, a QSPR study related to the ISD_a index in polyaromatic hydrocarbons is performed using experimental data. First, we determine the value of a that maximizes the Pearson's correlation coefficient between this index, and each of the studied physico-chemical properties. Finally, models for these properties are constructed using the simple linear regression method. A discussion of the results obtained is presented in Section 4, and some open problems for future research on this topic are raised.

In this research, $G = (V(G), E(G))$ denotes an undirected finite simple graph without isolated vertices. By n, m, Δ and δ, we denote the cardinality of the set of vertices of G, the cardinality of the set of edges of G, its maximum degree and its minimum degree, respectively. Thus, we have $1 \leq \delta \leq \Delta < n$. We denote by $N(u)$ the set of neighbors of the vertex $u \in V(G)$.

2. Extremal problems

Suppose $\delta < \Delta$, we say that a graph G is (δ, Δ)-*quasi-regular* if it contains a vertex w, such that $\delta = d_w$ and $\Delta = d_z$ for every $z \in V(G) \setminus \{w\}$; G is (δ, Δ)-*pseudo-regular* if it contains a vertex w, such that $\Delta = d_w$ and $\delta = d_z$ for every $z \in V(G) \setminus \{w\}$.

In [31] appears the following result.

Lemma 1. *Let k be an integer, such that* $2 \leq k < n$.

(1) *If nk is even, then there exists a k-regular graph that is connected and has n vertices.*

(2) *If nk is odd, then there exist a* $(k, k-1)$*-quasi-regular and a connected* $(k+1, k)$*-pseudo-regular graphs, which are connected and have n vertices.*

The following result is basic to the development of this work.

Lemma 2. *For each* $a < 0$*, the function* $f : \mathbb{R}^+ \times \mathbb{R}^+ \to \mathbb{R}^+$ *given by*

$$f(x, y) = \frac{1}{x^a + y^a}$$

is strictly increasing in each variable.

Proof. Since $a < 0$, we have

$$\frac{\partial f}{\partial x}(x, y) = \frac{-a x^{a-1}}{(x^a + y^a)^2} > 0.$$

Then, f is a strictly increasing function in x, and since f is symmetric, it is also strictly decreasing in y.

Using Lemma 2, we obtain the following result.

Proposition 3. *If G is a graph,* $u, v \in V(G)$ *with* $uv \notin E(G)$*, and* $a < 0$*, then* $ISD_a(G \cup \{uv\}) > ISD_a(G)$.

Given an integer number $n \geq 2$, let $\mathcal{G}(n)$ (respectively, $\mathcal{G}_c(n)$) be the set of graphs (respectively, connected graphs) with n vertices.

Next, given integer numbers $1 \leq \delta \leq \Delta < n$, we are going to define the following classes of graphs: let $\mathcal{H}(n, \delta)$ (respectively, $\mathcal{H}_c(n, \delta)$) be the graphs (respectively, connected graphs) with n vertices and minimum degree δ, and let $\mathcal{I}(n, \Delta)$ (respectively, $\mathcal{I}_c(n, \Delta)$) be the graphs (respectively, connected graphs) with maximum degree Δ and n vertices.

First, let us state an optimization result for the ISD_a index on $\mathcal{G}_c(n)$ and $\mathcal{G}(n)$ (see [32]).

Proposition 4. *Consider* $a < 0$ *and an integer* $n \geq 2$.

(1) *The graph that maximizes the* ISD_a *index on* $\mathcal{G}_c(n)$ *or* $\mathcal{G}(n)$ *is unique and given by the complete graph* K_n.

(2) *If a graph minimizes the* ISD_a *index on* $\mathcal{G}_c(n)$*, then it is a tree.*

(3) *If n is even, then the graph that minimizes the* ISD_a *index on* $\mathcal{G}(n)$ *is unique and given by the union of* $n/2$ *paths* P_2*. If n is odd, then the graph that minimizes the* ISD_a *index on* $\mathcal{G}(n)$ *is unique and given by the union of* $(n-3)/2$ *paths* P_2 *with a path* P_3.

Proof. Let G be a graph with n vertices, m edges and minimum degree δ.
Items (1) and (2) follow directly from Proposition 3.
For the proof of item (3), we first assume that n is even. For any graph $G \in \mathcal{G}(n)$ Lemma 2 gives

$$ISD_\alpha(G) = \sum_{uv\in E(G)} \frac{1}{d_u^a + d_v^a} \geq \sum_{uv\in E(G)} \frac{1}{1^a + 1^a} = \frac{m}{2},$$

and the equality is attained if, and only if, $\{d_u, d_v\} = \{1\}$ for each $uv \in E(G)$, i.e., G is the union of $n/2$ path graphs P_2.
Now, we assume that n is odd. If $d_u = 1$ for each $u \in V(G)$, handshaking lemma gives $2m = n$, a contradiction. So, there exists $w \in V(G)$, such that $d_w \geq 2$. Let $N(w)$ be the set of neighbors of the vertex w, from Lemma 2, we obtain

$$\begin{aligned} ISD_\alpha(G) &= \sum_{uv\in E(G),u,v\neq w} \frac{1}{d_u^a + d_v^a} + \sum_{u\in N(w)} \frac{1}{d_u^a + d_w^a} \\ &\geq \sum_{uv\in E(G),u,v\neq w} \frac{1}{1^a + 1^a} + \sum_{u\in N(w)} \frac{1}{1^a + 2^a} \\ &\geq \frac{m-2}{2} + \frac{2}{1+2^a}, \end{aligned}$$

and the equality is attained if, and only if, $d_u = 1$ for each $u \in V(G) \setminus w$ and $d_w = 2$. Hence, G is the union of $(n-3)/2$ path graphs P_2 and a path graph P_3.

Proposition 4 allows to obtain the following inequalities.

Theorem 5. *Consider a graph G with n vertices and a negative constant a.*
(1) *Then,*

$$ISD_a(G) \leq \frac{1}{4}\, n(n-1)^{1-a},$$

and equality holds if, and only if, G is the complete graph K_n.
(2) *If n is even, then*

$$ISD_a(G) \geq \frac{1}{4}\, n,$$

and equality holds if, and only if, G is the union of $n/2$ path graphs P_2.
(3) *If n is odd, then*

$$ISD_a(G) \geq \frac{1}{4}\,(n-3) + \frac{2}{1+2^a}\,,$$

and equality holds if, and only if, G is the union of a path graph P_3 and $(n-3)/2$ path graphs P_2.

Proof. Proposition 4 gives

$$ISD_a(G) \leq ISD_a(K_n) = \sum_{uv\in E(K_n)} \frac{1}{d_u^a + d_v^a} = \frac{n(n-1)}{2}\,\frac{1}{2(n-1)^a} = \frac{1}{4}\, n(n-1)^{1-a}.$$

This argument gives that the bound is attained if, and only if, G is the complete graph K_n. Hence, item (1) holds.

Suppose G has minimum degree δ. If n is even, handshaking lemma gives $2m \geq n\delta \geq n$, using this and the proof of Proposition 4, we have

$$ISD_a(G) \geq \frac{m}{2} \geq \frac{n}{4},$$

and equality holds if, and only if, G is the union of $n/2$ path graphs P_2. This gives item (2).
If n is odd, handshaking lemma gives $2m \geq (n-1)\delta + 2 \geq n+1$, using this and the proof of Proposition 4, we have

$$ISD_a(G) \geq \frac{m-2}{2} + \frac{2}{1+2^a} \geq \frac{\frac{n+1}{2}-2}{2} + \frac{2}{1+2^a} = \frac{n-3}{4} + \frac{2}{1+2^a},$$

and equality holds if, and only if, G is the union of a path graph P_3 and $(n-3)/2$ path graphs P_2. This gives item (3).

Fix positive integers $1 \leq \delta < n$. Let K_n^δ be the n-vertex graph with minimum and maximum degrees δ and $n-1$, respectively, obtained from K_{n-1} (the complete graph with $n-1$ vertices) and an additional vertex w, as follows: If we fix δ vertices $v_1, \dots, v_\delta \in V(K_{n-1})$, then the vertices of K_n^δ are w and the vertices of K_{n-1}, and the edges of K_n^δ are $\{v_1w, \dots, v_\delta w\}$ and the edges of K_{n-1}.

We consider now the optimization problem for the ISD_a index on $\mathcal{H}_c(n,\delta)$ and $\mathcal{H}(n,\delta)$.

Theorem 6. *Consider $a < 0$ and integers $1 \leq \delta < n$.*

(1) *Then, the graph in $\mathcal{H}_c(n,\delta)$ that maximizes the ISD_a index is unique and given by K_n^δ.*

(2) *If $\delta \geq 2$ and $n\delta$ is even, then all the graphs in $\mathcal{H}_c(n,\delta)$ that minimize ISD_a are the connected δ-regular graphs.*

(3) *If $\delta \geq 2$ and $n\delta$ is odd, then all the graphs in $\mathcal{H}_c(n,\delta)$ that minimize ISD_a are the connected $(\delta+1,\delta)$-pseudo-regular graphs.*

Proof. Given a graph $G \in \mathcal{H}_c(n,\delta) \setminus \{K_n^\delta\}$, fix any vertex $u \in V(G)$ with $d_u = \delta$. Since

$$G \neq G \cup \{vw : v, w \in V(G) \setminus \{u\} \text{ and } vw \notin E(G)\} = K_n^\delta,$$

Proposition 3 gives $ISD_a(K_n^\delta) > ISD_a(G)$. This proves item (1).

Handshaking lemma gives $2m \geq n\delta$.

Since $d_u \geq \delta$ for every $u \in V(G)$, Lemma 2 gives

$$ISD_a(G) = \sum_{uv\in E(G)} \frac{1}{d_u^a + d_v^a} \geq \sum_{uv\in E(G)} \frac{1}{2\delta^a} = \frac{m}{2\delta^a} \geq \frac{n\delta/2}{2\delta^a} = \frac{1}{4}\, n\delta^{1-a},$$

and the bound is attained if, and only if, $\delta = d_u$ for all $u \in V(G)$.

If δn is even, then Lemma 1 gives that there is a connected δ-regular graph with n vertices. Hence, the unique graphs in $\mathcal{H}_c(n,\delta)$ that minimize the ISD_a index are the connected δ-regular graphs.

If δn is odd, then handshaking lemma gives that there is no regular graph. Hence, there exists a vertex w with $d_w \geq \delta + 1$. Since $d_u \geq \delta$ for every $u \in V(G)$, handshaking lemma gives $2m \geq$

$(n-1)\delta + \delta + 1 = n\delta + 1$. Lemma 2 gives

$$
\begin{aligned}
ISD_a(G) &= \sum_{u \in N(w)} \frac{1}{d_u^a + d_w^a} + \sum_{uv \in E(G), u,v \neq w} \frac{1}{d_u^a + d_v^a} \\
&\geq \sum_{u \in N(w)} \frac{1}{\delta^a + (\delta+1)^a} + \sum_{uv \in E(G), u,v \neq w} \frac{1}{2\delta^a} \\
&\geq \frac{\delta + 1}{\delta^a + (\delta+1)^a} + \frac{m - \delta - 1}{2\delta^a} \\
&\geq \frac{\delta + 1}{\delta^a + (\delta+1)^a} + \frac{(n\delta + 1)/2 - \delta - 1}{2\delta^a},
\end{aligned}
$$

and the bound is attained if, and only if, $d_u = \delta$ for all $u \in V(G) \setminus \{w\}$, and $d_w = \delta + 1$. Lemma 1 gives that there is a connected $(\delta + 1, \delta)$-pseudo-regular graph with n vertices. Therefore, the unique graphs in $\mathcal{H}_c(n, \delta)$ that minimize the ISD_a index are the connected $(\delta + 1, \delta)$-pseudo-regular graphs.

Remark 1. *If we replace $\mathcal{H}_c(n, \delta)$ with $\mathcal{H}(n, \delta)$ everywhere in the statement of Theorem 6, then the argument in its proof gives that the same conclusions hold if we remove everywhere the word "connected".*

Theorem 6 and Remark 1 have the following consequence.

Proposition 7. *Consider a graph G with minimum degree δ and n vertices, and a negative constant a.*

(1) *Then,*

$$
ISD_a(G) \leq \frac{(n - \delta - 1)(n - \delta - 2)}{4(n-2)^a} + \frac{\delta}{\delta^a + (n-1)^a} + \frac{\delta(\delta - 1)}{4(n-1)^a} + \frac{\delta(n - \delta - 1)}{(n-2)^a + (n-1)^a},
$$

and the bound is attained if, and only if, G is isomorphic to K_n^δ.

(2) *If $\delta \geq 2$ and δn is even, then*

$$
ISD_a(G) \geq \frac{1}{4} n \delta^{1-a},
$$

and the bound is attained if, and only if, G is δ-regular.

(3) *If $\delta \geq 2$ and $n\delta$ is odd, then*

$$
ISD_a(G) \geq \frac{\delta(n-2) - 1}{4\delta^a} + \frac{\delta + 1}{\delta^a + (\delta + 1)^a},
$$

and the bound is attained if, and only if, G is $(\delta + 1, \delta)$-pseudo-regular.

Let us deal with the optimization problem for the ISD_a index on $\mathcal{I}_c(n, \Delta)$.

Theorem 8. *Consider $a < 0$ and integers $2 \leq \Delta < n$.*

(1) *If $n\Delta$ is even, then all the graphs that maximize ISD_a on $\mathcal{I}_c(n, \Delta)$ are the connected Δ-regular graphs.*

(2) *If $n\Delta$ is odd, then all the graphs that maximize ISD_a on $\mathcal{I}_c(n, \Delta)$ are the connected $(\Delta, \Delta - 1)$-quasi-regular graphs.*

(3) *If a graph minimizes ISD_a on $\mathcal{I}_c(n, \Delta)$, then it is a tree.*

Proof. Handshaking lemma gives $2m \le n\Delta$. Since $d_u \le \Delta$ for every $u \in V(G)$, Lemma 2 gives

$$ISD_a(G) = \sum_{uv \in E(G)} \frac{1}{d_u^a + d_v^a} \le \sum_{uv \in E(G)} \frac{1}{2\Delta^a} = \frac{m}{2\Delta^a} \le \frac{n\Delta/2}{2\Delta^a} = \frac{1}{4}\, n\Delta^{1-a},$$

and the bound is attained if, and only if, $\Delta = d_u$ for all $u \in V(G)$.

If $n\Delta$ is even, then Lemma 1 gives that there is a connected Δ-regular graph with n vertices. Hence, the unique graphs in $\mathcal{I}_c(n, \Delta)$ that maximize the ISD_a index are the connected Δ-regular graphs.

If $n\Delta$ is odd, then handshaking lemma gives that there is no regular graph in $\mathcal{I}_c(n, \Delta)$. Let $G \in \mathcal{I}_c(n, \Delta)$. Hence, there exists a vertex w with $d_w \le \Delta - 1$. Then, $2m \le \Delta(n - 1) + \Delta - 1 = \Delta n - 1$. Lemma 2 gives

$$\begin{aligned}
ISD_a(G) &= \sum_{u \in N(w)} \frac{1}{d_u^a + d_w^a} + \sum_{uv \in E(G), u,v \ne w} \frac{1}{d_u^a + d_v^a} \\
&\le \sum_{u \in N(w)} \frac{1}{\Delta^a + (\Delta - 1)^a} + \sum_{uv \in E(G), u,v \ne w} \frac{1}{2\Delta^a} \\
&\le \frac{\Delta - 1}{\Delta^a + (\Delta - 1)^a} + \frac{m - \Delta + 1}{2\Delta^a} \\
&\le \frac{\Delta - 1}{\Delta^a + (\Delta - 1)^a} + \frac{(\Delta n - 1)/2 - \Delta + 1}{2\Delta^a},
\end{aligned}$$

and the bound is attained if, and only if, $d_u = \Delta$ for all $u \in V(G) \setminus \{w\}$, and $d_w = \Delta - 1$. Lemma 1 gives that there is a connected $(\Delta, \Delta - 1)$-quasi-regular graph with n vertices. Therefore, the unique graphs in $\mathcal{I}_c(n, \delta)$ that maximize the ISD_a index are the connected $(\Delta, \Delta - 1)$-quasi-regular graphs.

Given any graph $G \in \mathcal{I}_c(n, \Delta)$ which is not a tree, fix any vertex $u \in V(G)$ with $d_u = \Delta$. Since G is not a tree, there exists a cycle C in G. Since C has at least three edges, there exists $vw \in E(G) \cap C$, such that $u \notin \{v, w\}$. Since vw is contained in a cycle of G, then $G \setminus \{vw\}$ is a connected graph. Thus, $G \setminus \{vw\} \in \mathcal{I}_c(n, \Delta)$ and Proposition 3 gives $ISD_a(G) > ISD_a(G \setminus \{vw\})$. By iterating this argument, we obtain that if a graph minimizes the ISD_a index on $\mathcal{I}_c(n, \Delta)$, then it is a tree.

The following result deals with the optimization problem for the ISD_a index on $\mathcal{I}(n, \Delta)$.

Theorem 9. *Consider $a < 0$ and integers $2 \le \Delta < n$.*

(1) *If $n\Delta$ is even, then all the graphs that maximize the ISD_a index on $\mathcal{I}(n, \Delta)$ are the Δ-regular graphs.*

(2) *If $n\Delta$ is odd, then all the graphs that maximize the ISD_a index on $\mathcal{I}(n, \Delta)$ are the $(\Delta, \Delta - 1)$-quasi-regular graphs.*

(3) *If $n - \Delta$ is odd, then the graph that minimizes the ISD_a index on $\mathcal{I}(n, \Delta)$ is unique and given by the union of the star graph $S_{\Delta+1}$ and $(n - \Delta - 1)/2$ path graphs P_2.*

(4) *If $n = \Delta + 2$, then the graph that minimizes the ISD_a index on $\mathcal{I}(n, \Delta)$ is unique and given by the star graph $S_{\Delta+1}$ with an additional edge attached to a vertex of degree 1 in $S_{\Delta+1}$.*

(5) *If $n \ge \Delta + 4$ and $n - \Delta$ is even, then the graph that minimizes the ISD_a index on $\mathcal{I}(n, \Delta)$ is unique and given by the union of the star graph $S_{\Delta+1}$, $(n - \Delta - 4)/2$ path graphs P_2 and a path graph P_3.*

Proof. The argument in Theorem 8 gives directly items (1) and (2).

Let $G \in \mathcal{I}(n, \Delta)$ and $w \in V(G)$ a vertex with $d_w = \Delta$.

Assume first that $n - \Delta$ is odd. Handshaking lemma gives $2m \geq n - 1 + \Delta$. Note that $n - 1 + \Delta = n - \Delta + 2\Delta - 1$ is even. Lemma 2 gives

$$\begin{aligned} ISD_a(G) &= \sum_{u \in N(w)} \frac{1}{d_u^a + d_w^a} + \sum_{uv \in E(G), u,v \neq w} \frac{1}{d_u^a + d_v^a} \\ &\geq \sum_{u \in N(w)} \frac{1}{1^a + \Delta^a} + \sum_{uv \in E(G), u,v \neq w} \frac{1}{1^a + 1^a} \\ &= \frac{\Delta}{1 + \Delta^a} + \frac{m - \Delta}{2} \\ &\geq \frac{\Delta}{1 + \Delta^a} + \frac{(n - 1 + \Delta)/2 - \Delta}{2} \\ &= \frac{\Delta}{1 + \Delta^a} + \frac{n - \Delta - 1}{4}, \end{aligned}$$

and the bound is attained if, and only if, $1 = d_u$ for all $u \in V(G) \setminus \{w\}$, i.e., G is the union of the star graph $S_{\Delta+1}$ and $(n - \Delta - 1)/2$ path graphs P_2.

Assume now that $n = \Delta + 2$. Let $z \in V(G) \setminus N(w)$ be the vertex with $V(G) = \{w, z\} \cup N(w)$. Choose $p \in N(z)$; since $z \notin N(w)$, we have $p \in N(w)$ and so, $d_p \geq 2$. Handshaking lemma gives $2m \geq (n - 2) + \Delta + 2 = n + \Delta$. Lemma 2 gives

$$\begin{aligned} ISD_a(G) &= \sum_{u \in N(w)} \frac{1}{d_u^a + d_w^a} + \sum_{uv \in E(G), u,v \neq w} \frac{1}{d_u^a + d_v^a} \\ &\geq \frac{\Delta - 1}{1 + \Delta^a} + \frac{1}{2^a + \Delta^a} + \frac{1}{1 + 2^a}, \end{aligned}$$

and the bound is attained if, and only if, $1 = d_u$ for all $u \in V(G) \setminus \{w, p\}$ and $d_p = 2$, i.e., G is the star graph $S_{\Delta+1}$ with an additional edge attached to a vertex of degree 1 in $S_{\Delta+1}$.

Assume that $n \geq \Delta + 4$ and $n - \Delta$ is even. If $d_u = 1$ for every $u \in V(G) \setminus \{w\}$, then handshaking lemma gives $2m = n - 1 + \Delta$, a contradiction since $n - 1 + \Delta = n - \Delta + 2\Delta - 1$ is odd. Thus, there exists a vertex $p \in V(G) \setminus \{w\}$ with $d_p \geq 2$. Handshaking lemma gives $2m \geq (n - 2) + 2 + \Delta = n + \Delta$.

If $p \notin N(w)$, then Lemma 2 gives

$$\begin{aligned} ISD_a(G) &= \sum_{u \in N(w)} \frac{1}{d_u^a + d_w^a} + \sum_{u \in N(p)} \frac{1}{d_u^a + d_p^a} + \sum_{uv \in E(G), u,v \notin \{w,p\}} \frac{1}{d_u^a + d_v^a} \\ &\geq \sum_{u \in N(w)} \frac{1}{1^a + \Delta^a} + \sum_{u \in N(p)} \frac{1}{1^a + 2^a} + \sum_{uv \in E(G), u,v \notin \{w,p\}} \frac{1}{1^a + 1^a} \\ &\geq \frac{\Delta}{1 + \Delta^a} + \frac{2}{1 + 2^a} + \frac{m - \Delta - 2}{2} \\ &\geq \frac{\Delta}{1 + \Delta^a} + \frac{2}{1 + 2^a} + \frac{(n + \Delta)/2 - \Delta - 2}{2} \\ &= \frac{\Delta}{1 + \Delta^a} + \frac{2}{1 + 2^a} + \frac{n - \Delta - 4}{4}, \end{aligned}$$

and the bound is attained if, and only if, $d_u = 1$ for all $u \in V(G) \setminus \{w, p\}$, and $d_p = 2$, i.e., G is the union of the star graph $S_{\Delta+1}$, $(n - \Delta - 4)/2$ path graphs P_2 and a path graph P_3.

If $p \in N(w)$, then

$$\begin{aligned}
ISD_a(G) &= \sum_{u\in N(w)\setminus\{p\}} \frac{1}{d_u^a + d_w^a} + \sum_{u\in N(p)\setminus\{w\}} \frac{1}{d_u^a + d_p^a} + \frac{1}{d_p^a + d_w^a} + \sum_{uv\in E(G),u,v\notin\{w,p\}} \frac{1}{d_u^a + d_v^a} \\
&\geq \sum_{u\in N(w)\setminus\{p\}} \frac{1}{1^a + \Delta^a} + \sum_{u\in N(p)\setminus\{w\}} \frac{1}{1^a + d_p^a} + \frac{1}{d_p^a + \Delta^a} + \sum_{uv\in E(G),u,v\notin\{w,p\}} \frac{1}{1^a + 1^a} \\
&\geq \frac{\Delta - 1}{1 + \Delta^a} + \frac{1}{1 + 2^a} + \frac{1}{2^a + \Delta^a} + \frac{m - \Delta - 1}{2} \\
&\geq \frac{\Delta - 1}{1 + \Delta^a} + \frac{1}{1 + 2^a} + \frac{1}{2^a + \Delta^a} + \frac{(n + \Delta)/2 - \Delta - 1}{2} \\
&= \frac{\Delta - 1}{1 + \Delta^a} + \frac{1}{1 + 2^a} + \frac{1}{2^a + \Delta^a} + \frac{n - \Delta - 2}{4}\,.
\end{aligned}$$

Hence, in order to finish the proof of item (5), it suffices to show that

$$\frac{\Delta - 1}{1 + \Delta^a} + \frac{1}{1 + 2^a} + \frac{1}{2^a + \Delta^a} + \frac{n - \Delta - 2}{4} > \frac{\Delta}{1 + \Delta^a} + \frac{2}{1 + 2^a} + \frac{n - \Delta - 4}{4}\,.$$

We have

$$\begin{gathered}
(1 - 2^a)(1 - \Delta^a) > 0, \\
1 + 2^a\Delta^a > 2^a + \Delta^a, \\
2^a\Delta^a + \Delta^a + 2^a + 1 > 2(2^a + \Delta^a), \\
(\Delta^a + 1)(1 + 2^a)(2 + 2^a + \Delta^a) > 2(2^a + \Delta^a)(2^a + \Delta^a + 2), \\
\frac{1}{2^a + \Delta^a} + \frac{1}{2} > \frac{1}{1 + \Delta^a} + \frac{1}{1 + 2^a}\,, \\
\frac{\Delta - 1}{1 + \Delta^a} + \frac{1}{1 + 2^a} + \frac{1}{2^a + \Delta^a} + \frac{n - \Delta - 2}{4} > \frac{\Delta}{1 + \Delta^a} + \frac{2}{1 + 2^a} + \frac{n - \Delta - 4}{4}\,,
\end{gathered}$$

and so, (5) holds.

Remark 2. *Note that the case $\Delta = 1$ in Theorem 9 is trivial: if $\Delta = 1$, then G is a union of isolated edges.*

Also, we can state the following inequalities.

Theorem 10. *Consider a graph G with maximum degree Δ and n vertices, and a negative constant a.*

(1) *If $n\Delta$ is even, then*

$$ISD_a(G) \leq \frac{1}{4}\, n\Delta^{1-a},$$

and the bound is attained if, and only if, G is a regular graph.

(2) *If $n\Delta$ is odd, then*

$$ISD_a(G) \leq \frac{\Delta - 1}{\Delta^a + (\Delta - 1)^a} + \frac{\Delta(n - 2) + 1}{4\Delta^a}\,,$$

and the bound is attained if, and only if, G is a $(\Delta, \Delta - 1)$-quasi-regular graph.

(3) *If $n - \Delta$ is odd, then*

$$ISD_a(G) \geq \frac{\Delta}{1 + \Delta^a} + \frac{n - \Delta - 1}{4}\,,$$

and the bound is attained if, and only if, G is the union of the star graph $S_{\Delta+1}$ *and* $(n - \Delta - 1)/2$ *path graphs* P_2.

(4) *If* $n = \Delta + 2$, *then*

$$ISD_a(G) \geq \frac{\Delta - 1}{1 + \Delta^a} + \frac{1}{2^a + \Delta^a} + \frac{1}{1 + 2^a},$$

and the bound is attained if, and only if, G is the star graph $S_{\Delta+1}$ *with an additional edge attached to a vertex of degree* 1 *in* $S_{\Delta+1}$.

(5) *If* $n \geq \Delta + 4$ *and* $n - \Delta$ *is even, then*

$$ISD_a(G) \geq \frac{\Delta}{1 + \Delta^a} + \frac{2}{1 + 2^a} + \frac{n - \Delta - 4}{4},$$

and the bound is attained if, and only if, G is the union of the star graph $S_{\Delta+1}$, $(n-\Delta-4)/2$ *path graphs* P_2 *and a path graph* P_3.

Proof. The argument in the proof of Theorem 8 gives items (1) and (2), since the variable inverse sum deg index of a regular graph is

$$\frac{1}{4} n\Delta^{1-a},$$

and the ISD_a index of a $(\Delta, \Delta - 1)$-quasi-regular graph is

$$\frac{\Delta - 1}{\Delta^a + (\Delta - 1)^a} + \frac{\Delta(n - 2) + 1}{4\Delta^a}.$$

The argument in the proof of Theorem 9 gives directly items (3)–(5).

3. QSPR study of ISD_a on polyaromatic hydrocarbons

The variable inverse sum deg index $ISD_{-1.950}$ was selected in [33] as a significant predictor of standard enthalpy of formation for octane isomers. In this section, we will test the predictive power of the ISD_a index using experimental data on three physicochemical properties of 82 polyaromatic hydrocarbons (PAH). The properties studied are the melting point (MP), boiling point (BP) and octanol-water partition coefficient (LogP) (the experimental data were obtained from [34]). In order to obtain the values of the ISD_a index, we constructed the hydrogen-suppressed graph of each molecule, then we use a program of our own elaboration to compute the index for each value of a analyzed.

We calculated the Pearson's correlation coefficient r between the three analyzed properties and the ISD_a index, for values of a in the interval $[-5, 5]$ with a spacing of 0.01; the results are shown in Figure 1. The dashed red line indicates the value of a that maximizes r.

Figure 2 shows the *ISDa* index (for values of a that maximize r) vs. the studied properties of PAH. In addition, in Figure 2, we test the following linear regression models (red lines)

$$\begin{aligned} MP &= 31.54\, ISD_{0.15} - 121.15 \\ BP &= 58.94\, ISD_{0.39} - 13.35 \\ LogP &= 0.68\, ISD_{0.63} + 1.55. \end{aligned}$$

Table 1 summarizes the statistical and regression parameters of these models.

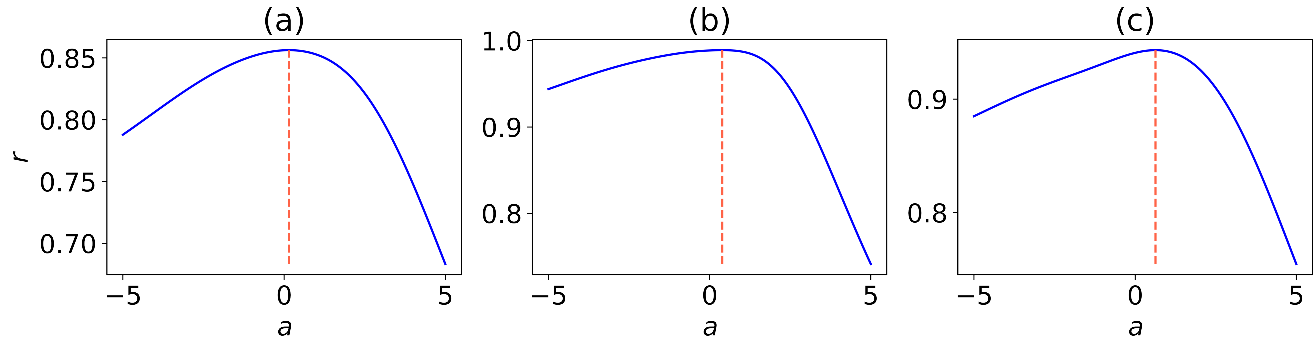

Figure 1. Pearson's correlation coefficient r between the ISD_a index and the following properties of polyaromatic hydrocarbons (a) melting point (MP), (b) boiling point (BP), and (c) octanol-water partition coefficient (LogP). Red dashed vertical line indicates the value of a for which r is maximized.

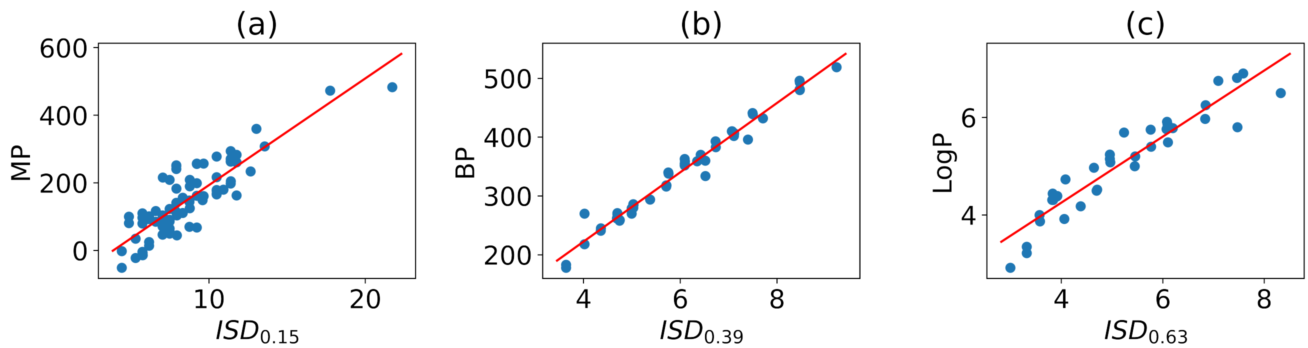

Figure 2. Properties of polyaromatic hydrocarbons vs. ISD_a index for the values of a that maximize the correlation coefficient r: (a) $a = 0.15$, (b) $a = 0.39$, and (c) $a = 0.63$. Red lines are the regression models obtained.

Table 1. Parameters of the linear QSPR models. Here, r, c, m, SE, F, and SF are the correlation coefficient, intercept, slope, standard error, F-test, and statistical significance, respectively.

Property	a	r	c	m	SE	F	SF
MP	0.15	0.856	−122.15	31.54	54.61	214.47	4.31×10^{-24}
BP	0.39	0.989	−13.35	58.94	12.42	2272.86	5.69×10^{-44}
LogP	0.63	0.943	1.55	0.68	0.34	282.04	2.53×10^{-18}

4. Conclusions

Motivated by a paper of Vukičević [1], and based on the practical applications found for the variable inverse sum deg index ISD_a, we focus our research on the study of optimal graphs associated with ISD_a, when $a < 0$. In this direction, it is wise to study the extremal properties of ISD_a, when $a < 0$ in general graphs. Specifically, in this paper, we characterize the graphs with extremal values in the following significant classes of graphs with a fixed number of vertices:

- graphs with a fixed minimum degree;
- connected graphs with a fixed minimum degree;
- graphs with a fixed maximum degree;
- connected graphs with a fixed maximum degree.

From the QSPR study performed on polyaromatic hydrocarbons, it can be concluded that the ISD_a index presents a strong correlation with the boiling point and octanol-water partition coefficient properties, with maximum values of r higher than 0.98 and 0.94, respectively. Further, the melting point property presents some correlation with the ISD_a index with maximum value of r close to 0.85.

For future research, we suggests:

- To study the extreme problems for the ISD_a index for values of $a > 0$.
- To consider the problem of finding which tree/trees with n vertices (with a fixed maximum degree or not) minimize the index ISD_a ($a < 0$).
- To analyze the behavior of the ISD_a index in other important families of graphs, such as graph products and graph operators.
- To explore the mathematical properties and possible applications of the exponential extension of the ISD_a index.
- To study the predictive power of this index on other physicochemical properties of PAH, and on other classes of molecules.

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Conflict of interest

The authors declare there are no conflicts of interest.

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