Analytical and computational study of the variable inverse sum deg index

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Abstract. A large number of graph invariants of the form \(\sum_{uv \in E(G)} F(d_u, d_v)\) are studied in mathematical chemistry, where \(uv\) denotes the edge of the graph \(G\) connecting the vertices \(u\) and \(v\), 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 applicative properties. The aim of this paper is to obtain new inequalities for the variable inverse sum deg index, and to characterize graphs extremal with respect to them. Some of these inequalities generalize and improve previous results for the inverse sum indeg index. In addition, we computationally validate some of the obtained inequalities on ensembles of random graphs and show that the ratio \(\langle ISD_a(G) \rangle / n\) (\(n\) being the order of the graph) depends only on the average degree \(\langle d \rangle\).

Keywords. variable inverse sum deg index · inverse sum indeg index · optimization on graphs · degree–based topological index

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1 Introduction

Topological indices are parameters associated with chemical compounds that associate the chemical structure with several physical, chemical or biological properties.

A family of degree–based topological indices, named Adriatic indices, was put forward in [37,38]. Twenty of them were selected as significant predictors. One of them, the inverse sum indeg index, $ISI$, was singled out in [37,38] as a significant predictor of total surface area of octane isomers. This index is defined as

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

where $uv$ denotes the edge of the graph $G$ connecting the vertices $u$ and $v$, and $d_u$ is the degree of the vertex $u$. In the last years there is an increasing interest in the mathematical properties of this index (see, e.g., [6,11,13,14,21,26,30]).

We study here the properties of the variable inverse sum deg index defined, for each $a \in \mathbb{R}$, as

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

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

The variable inverse sum deg index $ISD_{-1.950}$ was selected in [39] as a significant predictor of standard enthalpy of formation.

The idea behind the variable molecular descriptors is that the variables are determined during the regression so that the standard error of estimate for a particular studied property is as small as possible (see, e.g., [20]).

The aim of this paper is to obtain new inequalities for the variable inverse sum deg index, and to characterize graphs extremal with respect to them. Some of these inequalities generalize and improve previous results for the inverse sum indeg index. Also, we want to remark that many previous results are proved for connected graphs, but our inequalities hold for both connected and non-connected graphs.

Throughout this paper, $G = (V(G), E(G))$ denotes an undirected finite simple (without multiple edges and loops) graph without isolated vertices. We denote by $n$, $m$, $\Delta$ and $\delta$ 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 Inequalities for the ISD\(a\) index

**Proposition 1** If \(G\) is a graph with minimum degree \(\delta\), maximum degree \(\Delta\) and \(m\) edges, and \(a \in \mathbb{R}\), then

\[
\frac{m}{2\Delta^a} \leq ISD_a(G) \leq \frac{m}{2\delta^a}, \quad \text{if } a > 0, \\
\frac{m}{2\delta^a} \leq ISD_a(G) \leq \frac{m}{2\Delta^a}, \quad \text{if } a < 0.
\]

The equality in each bound is attained if and only if \(G\) is regular.

**Proof** If \(a > 0\), then \(2\delta^a \leq d_u^a + d_v^a \leq 2\Delta^a\) and

\[
ISD_a(G) = \sum_{uv \in E(G)} \frac{1}{d_u^a + d_v^a} \leq \sum_{uv \in E(G)} \frac{1}{2\delta^a} = \frac{m}{2\delta^a},
\]

\[
ISD_a(G) = \sum_{uv \in E(G)} \frac{1}{d_u^a + d_v^a} \geq \sum_{uv \in E(G)} \frac{1}{2\Delta^a} = \frac{m}{2\Delta^a}.
\]

If \(a < 0\), then the previous argument gives the converse inequalities.

If \(G\) is a regular graph, then the lower and upper bounds are the same, and they are equal to \(ISD_a(G)\).

Assume now that the equality in some bound is attained. Thus, by the previous argument we have either \(d_u = d_v = \delta\) for every \(uv \in E(G)\), or \(d_u = d_v = \Delta\) for every \(uv \in E(G)\). Hence, \(G\) is regular.

In 1998 Bollobás and Erdős [3] generalized the Randić index by replacing \(1/2\) by any real number. Thus, for \(a \in \mathbb{R} \setminus \{0\}\), the general Randić index of a graph \(G\) is defined as

\[
R_a(G) = \sum_{uv \in E(G)} (d_u d_v)^a.
\]

The general Randić index, also called variable Zagreb index in 2004 by Milicević and Nikolić [20], has been extensively studied [15]. Note that \(R_{-1/2}\) is the usual Randić index, \(R_1\) is the second Zagreb index \(M_2\), \(R_{-1}\) is the modified Zagreb index [24], etc. In Randić’s original paper [27], in addition to the particular case \(a = -1/2\), also the index with \(a = -1\) was briefly considered.

The next result relates the \(ISD_a\) and \(R_{-a}\) indices.

**Theorem 1** If \(G\) is a graph with minimum degree \(\delta\) and maximum degree \(\Delta\), and \(a \in \mathbb{R}\), then

\[
\frac{1}{2} \delta^a R_{-a}(G) \leq ISD_a(G) \leq \frac{1}{2} \Delta^a R_{-a}(G), \quad \text{if } a > 0, \\
\frac{1}{2} \Delta^a R_{-a}(G) \leq ISD_a(G) \leq \frac{1}{2} \delta^a R_{-a}(G), \quad \text{if } a < 0.
\]

The equality in each bound is attained if and only if \(G\) is regular.
Proof We have

\[ ISD_a(G) = \sum_{uv \in E(G)} \frac{1}{d_u^a + d_v^a} = \sum_{uv \in E(G)} \frac{(d_ud_v)^{-a}}{d_u^a + d_v^a} \]

If \( a > 0 \), then \( 2\Delta^{-a} \leq d_u^{-a} + d_v^{-a} \leq 2\delta^{-a} \), and

\[ \frac{1}{2} \delta^a R_{-a}(G) = \sum_{uv \in E(G)} \frac{(d_u d_v)^{-a}}{2\delta^{-a}} \leq \sum_{uv \in E(G)} \frac{(d_u d_v)^{-a}}{d_u^a + d_v^a} \leq \sum_{uv \in E(G)} \frac{(d_u d_v)^{-a}}{2\Delta^{-a}} = \frac{1}{2} \Delta^a R_{-a}(G) \]

If \( a < 0 \), then the previous argument gives the converse inequalities.

If \( G \) is a regular graph, then the lower and upper bounds are the same, and they are equal to \( ISD_a(G) \).

Assume now that the equality in some bound is attained. Thus, by the previous argument we have either \( d_u = d_v = \delta \) for every \( uv \in E(G) \), or \( d_u = d_v = \Delta \) for every \( uv \in E(G) \). Hence, \( G \) is regular.

The following result relates the \( ISD_a \) and \( ISD_{-a} \) indices.

**Theorem 2** If \( G \) is a graph with minimum degree \( \delta \) and maximum degree \( \Delta \), and \( a \in \mathbb{R} \), then

\[ \Delta^{-2a} ISD_{-a}(G) \leq ISD_a(G) \leq \delta^{-2a} ISD_{-a}(G), \quad \text{if } a > 0, \]

\[ \delta^{-2a} ISD_{-a}(G) \leq ISD_a(G) \leq \Delta^{-2a} ISD_{-a}(G), \quad \text{if } a < 0. \]

The equality in each bound is attained if and only if \( G \) is regular.

Proof We have

\[ ISD_a(G) = \sum_{uv \in E(G)} \frac{1}{d_u^a + d_v^a} = \sum_{uv \in E(G)} \frac{(d_ud_v)^{-a}}{d_u^a + d_v^a} \]

Similarly, we obtain the result if \( a > 0 \).

\[ \Delta^{-2a} ISD_{-a}(G) = \sum_{uv \in E(G)} \frac{\Delta^{-2a}}{d_u^a + d_v^a} \leq ISD_a(G) \]

\[ \leq \sum_{uv \in E(G)} \frac{\delta^{-2a}}{d_u^a + d_v^a} = \delta^{-2a} ISD_{-a}(G). \]

If \( a < 0 \), then the previous argument gives the converse inequalities.

If \( G \) is a regular graph, then the lower and upper bounds are the same, and they are equal to \( ISD_a(G) \).

If the equality in some bound is attained, by the previous argument we have either \( d_u = d_v = \delta \) for every \( uv \in E(G) \), or \( d_u = d_v = \Delta \) for every \( uv \in E(G) \). Therefore, \( G \) is regular.
The general sum-connectivity index was defined in [42] as
\[ \chi_a(G) = \sum_{uv \in E(G)} (d_u + d_v)^a. \]
Note that \( \chi_1 \) is the first Zagreb index \( M_1 \), \( 2\chi_{-1} \) is the harmonic index \( H \), \( \chi_{-1/2} \) is the sum-connectivity index \( \chi \), etc.

The following result relates the variable inverse sum deg and the general sum-connectivity indices.

**Theorem 3** If \( G \) is a graph and \( a \in \mathbb{R} \setminus \{0, 1\} \), then
\[ \chi_{-a}(G) < ISD_a(G) \leq 2^{a-1} \chi_{-a}(G), \quad \text{if } a > 1, \] (1)
\[ 2^{a-1} \chi_{-a}(G) \leq ISD_a(G) < \chi_{-a}(G), \quad \text{if } 0 < a < 1, \] (2)
\[ ISD_a(G) \leq 2^{a-1} \chi_{-a}(G), \quad \text{if } a < 0. \] (3)

The equality in the first or third upper bound or in the second lower bound is attained if and only if each connected component of \( G \) is regular.

**Proof** We want to compute the minimum and maximum values of the function \( f : \mathbb{R}^+ \times \mathbb{R}^+ \to \mathbb{R}^+ \) given by
\[ f(x, y) = \frac{(x + y)^a}{x^a + y^a}. \]
In order to do that, we are going to compute the extremal values of \( g(x, y) = (x + y)^a \) with the restrictions \( h(x, y) = x^a + y^a = 1, \ x, y > 0 \). If \( (x, y) \) is a critical point, then there exists \( \lambda \in \mathbb{R} \) such that
\[ a(x + y)^a - 1 = \lambda (x^a - 1), \]
and so, \( x = y \); this fact and the equality \( x^a + y^a = 1 \) give \( x = y = 2^{-1/a} \) and \( g(2^{-1/a}, 2^{-1/a}) = 2^{a-1} \).

If \( a > 1 \) and \( x \to 0^+ \) (respectively, \( y \to 0^+ \)), then \( y \to 1 \) (respectively, \( x \to 1 \)) and \( g(x, y) \to 1 \).

If \( a > 1 \), then \( 1 < g(x, y) \leq 2^{a-1} \) and the upper bound is attained if and only if \( x = y \). By homogeneity, we have \( 1 < f(x, y) \leq 2^{a-1} \) for every \( x, y > 0 \) and the upper bound is attained if and only if \( x = y \).

If \( 0 < a < 1 \), then \( 2^{a-1} \leq f(x, y) < 1 \) and the lower bound is attained if and only if \( x = y \). Thus, \( 2^{a-1} \leq f(x, y) < 1 \) for every \( x, y > 0 \) and the lower bound is attained if and only if \( x = y \).

If \( a < 0 \), then \( x, y > 1 \). If \( x \to 1^+ \) (respectively, \( y \to 1^+ \)), then \( y \to \infty \) (respectively, \( x \to \infty \)) and \( g(x, y) \to 0 \). Hence, \( 0 < g(x, y) \leq 2^{a-1} \) and the upper bound is attained if and only if \( x = y \). Thus, \( 0 \leq f(x, y) \leq 2^{a-1} \) for every \( x, y > 0 \) and the upper bound is attained if and only if \( x = y \).
Note that if $c_a \leq f(x, y) \leq C_a$, then
\[
\frac{1}{(d_u + d_v)^a} \leq \frac{c_a}{d_u^a + d_v^a} \leq \frac{1}{(d_u + d_v)^a}
\]
for every $uv \in E(G)$ and, consequently, $C_a \chi^-(G) \leq ISD_a(G) \leq C_a \chi^-(G)$. These facts give the inequalities.

If $G$ is a connected $\delta$-regular graph with $m$ edges, then
\[
2^{a-1} \chi^-(G) = 2^{a-1}(2\delta)^{-a}m = \frac{m}{2\delta^a} = ISD_a(G).
\]
By linearity, the equality $2^{a-1} \chi^-(G) = ISD_a(G)$ also holds if each connected component of $G$ is regular.

Assume now that the equality in the first or third upper bound or in the second lower bound is attained. Thus, the previous argument gives that $d_u = d_v$ for every $uv \in E(G)$ and, consequently, each connected component of $G$ is regular.

Note that Theorem 3 with $a = -1$, gives $ISI(G) \leq M_1(G)/4$, a known inequality (see [30, Theorem 4]). Hence, Theorem 3 generalizes [30, Theorem 4].

Remark 1 Note that if we take limits as $a \to 1$ in Theorem 3, then we obtain by continuity the trivial equality $ISD_1(G) = \chi^{-1}(G)$.

The geometric-arithmetic index was introduced in [40] as
\[
GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_ud_v}}{d_u + d_v}.
\]
Although it was introduced in 2009, there are many papers dealing with this index (see, e.g., [9], [10], [18], [22], [25], [28], [32], [33], [34], [40] and the references therein). The predicting ability of the $GA$ index compared with Randić index is reasonably better (see [9, Table 1]). The graphic in [9, Fig.7] (from [9, Table 2], [35]) shows that there exists a good linear correlation between $GA$ and the heat of formation of benzenoid hydrocarbons (the correlation coefficient is equal to 0.972). Furthermore, the improvement in prediction with $GA$ index comparing to Randić index in the case of standard enthalpy of vaporization is more than 9%. That is why one can think that $GA_1$ index should be considered in the QSPR/QSAR researches.

The following result relates the variable inverse sum deg and the geometric-arithmetic indices.

**Theorem 4** If $G$ is a graph and $a \in \mathbb{R}$, then
\[
ISD_a(G) \geq \frac{1}{2} \Delta^{-a}GA(G), \quad \text{if } a > 0,
\]
\[
ISD_a(G) \geq \frac{1}{2} \delta^{-a}GA(G), \quad \text{if } a < 0.
\]
The equality in each bound is attained if and only if $G$ is a regular graph.
Proof We are going to compute the minimum and maximum values of the function \( V : [\delta, \Delta] \times [\delta, \Delta] \to \mathbb{R}^+ \) given by

\[
V(x, y) = \frac{x + y}{2\sqrt{xy}(x^a + y^a)}.
\]

We have

\[
\frac{\partial V}{\partial x}(x, y) = \frac{x^{1/2}(x^a + y^a) - (x + y)(x^{a-1/2}(x^a + y^a) + x^{1/2}ay^{a-1})}{x(x^a + y^a)^2}
\]

\[
= 2x(x^a + y^a) - (x + y)(x^a + y^a + 2ax^a)
\]

\[
= \frac{(x - y)(x^a + y^a) - 2a(x + y)x^a}{4x^{3/2}y^{1/2}(x^a + y^a)^2}.
\]

Assume first that \( a > 0 \). By symmetry, we can assume that \( x \leq y \). Thus, \( \partial V/\partial x(x, y) < 0 \) for \( \delta \leq x \leq y \leq \Delta \), and so,

\[
V(x, y) \geq V(y, y) = \frac{1}{2y^a} \geq \frac{1}{2} \Delta^{-a},
\]

and the equality in the bound is attained if and only if \( x = y = \Delta \). Hence,

\[
ISD_a(G) = \sum_{uv \in E(G)} \frac{1}{d_u + d_v} \geq \frac{1}{2} \Delta^{-a} \sum_{uv \in E(G)} \frac{2\sqrt{d_ud_v}}{d_u + d_v} = \frac{1}{2} \Delta^{-a} GA(G),
\]

and the equality in the bound is attained if and only if \( d_u = d_v = \Delta \) for every \( uv \in E(G) \), i.e., \( G \) is a regular graph.

Assume now that \( a < 0 \). We can assume that \( y \leq x \). Thus, \( \partial V/\partial x(x, y) > 0 \) for \( \delta \leq y \leq x \leq \Delta \), and so,

\[
V(x, y) \geq V(y, y) = \frac{1}{2y^a} \geq \frac{1}{2} \delta^{-a},
\]

and the equality in the bound is attained if and only if \( x = y = \Delta \). Hence,

\[
ISD_a(G) = \sum_{uv \in E(G)} \frac{1}{d_u + d_v} \geq \frac{1}{2} \delta^{-a} \sum_{uv \in E(G)} \frac{2\sqrt{d_ud_v}}{d_u + d_v} = \frac{1}{2} \delta^{-a} AG(G),
\]

and the equality in the bound is attained if and only if \( d_u = d_v = \delta \) for every \( uv \in E(G) \), i.e., \( G \) is a regular graph.
As an inverse variant of the geometric-arithmetic index, in 2015, the arithmetic-geometric index was introduced in [31] as

$$AG(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}}.$$  

In [23] it is shown that the arithmetic-geometric index has a good predictive power for entropy of octane isomers. The paper [41] studied spectrum and energy of arithmetic-geometric matrix, in which the sum of all elements is equal to $2AG$. Other bounds of the arithmetic-geometric energy of graphs appeared in [12], [8]. The paper [36] studies optimal $AG$-graphs for several classes of graphs. In [4], [7], [23] and [29] there are more bounds on the $AG$ index.

The following result relates the variable inverse sum deg and the arithmetic-geometric indices.

**Theorem 5** If $G$ is a graph and $a \in \mathbb{R}$, then

$$ISD_a(G) \leq \frac{1}{2} \delta^{-a} AG(G), \quad \text{if } a > 0,$$

$$ISD_a(G) \leq \frac{1}{2} \Delta^{-a} AG(G), \quad \text{if } a < 0.$$  

The equality in each bound is attained if and only if $G$ is a regular graph.

**Proof** We are going to compute the minimum and maximum values of the function $U : [\delta, \Delta] \times [\delta, \Delta] \to \mathbb{R}^+$ given by

$$U(x, y) = \frac{2\sqrt{xy}}{(x+y)(x^a + y^a)}.$$  

We have

$$\frac{\partial U}{\partial x}(x, y) = \sqrt{y} \frac{x^{-1/2}(x+y)(x^a + y^a) - 2x^{1/2}(x^a + y^a + (x+y)ax^{a-1})}{(x+y)^2(x^a + y^a)^2}$$

$$= \sqrt{y} \frac{(x+y)(x^a + y^a) - 2(x(x^a + y^a) + (x+y)ax^a)}{\sqrt{x} (x+y)^2(x^a + y^a)^2}$$

$$= \sqrt{y} \frac{y-x)(x^a + y^a) - 2(x+y)ax^a}{\sqrt{x} (x+y)^2(x^a + y^a)^2}.$$  

Assume first that $a > 0$. By symmetry, we can assume that $x \geq y$. Thus, $\partial U/\partial x(x, y) < 0$ for $\delta \leq y \leq x \leq \Delta$, and so,

$$U(x, y) \leq U(y, y) = \frac{1}{2y^a} \leq \frac{1}{2} \delta^{-a},$$
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and the equality in the bound is attained if and only if \( x = y = \delta \). Hence,

\[
ISD_a(G) = \sum_{uv \in E(G)} \frac{1}{d_u^a + d_v^a} \leq \frac{1}{2} \delta^{-a} \frac{d_u + d_v}{2\sqrt{d_u d_v}} = \frac{1}{2} \delta^{-a} AG(G),
\]

and the equality in the bound is attained if and only if \( d_u = d_v = \delta \) for every \( uv \in E(G) \), i.e., \( G \) is a regular graph.

Assume now that \( a < 0 \). We can assume that \( x \leq y \). Thus, \( \partial U/\partial x(x,y) > 0 \) for \( \delta \leq x \leq y \leq \Delta \), and so,

\[
U(x,y) \leq U(y,y) = \frac{1}{2y^a} \leq \frac{1}{2} \Delta^{-a},
\]

and the equality in the bound is attained if and only if \( x = y = \Delta \). Hence,

\[
ISD_a(G) = \sum_{uv \in E(G)} \frac{1}{d_u^a + d_v^a} \leq \frac{1}{2} \Delta^{-a} \frac{d_u + d_v}{2\sqrt{d_u d_v}} = \frac{1}{2} \Delta^{-a} AG(G),
\]

and the equality in the bound is attained if and only if \( d_u = d_v = \Delta \) for every \( uv \in E(G) \), i.e., \( G \) is a regular graph.

Miličević and Nikolić defined in [20] the \textit{variable first Zagreb index} as

\[
M^a_1(G) = \sum_{u \in V(G)} d_u^a,
\]

with \( a \in \mathbb{R} \). Note that \( M^2_1 \) is the first Zagreb index \( M_1 \), \( M^{-1}_1 \) is the the inverse index \( ID \), \( M^{-1/2}_1 \) is the zeroth-order Randić index, \( M^0_1 \) is the forgotten index \( F \), etc.

\textbf{Theorem 6} If \( G \) is a graph with \( m \) edges, and \( a \in \mathbb{R} \), then

\[
ISD_a(G) + M^{a+1}_1(G) \geq \frac{5}{2} m, \quad \text{if } a > 0, \quad (4)
\]

\[
ISD_a(G) + M^{a+1}_1(G) \geq 2m, \quad \text{if } a < 0. \quad (5)
\]

The equality in the first bound is attained if and only if \( G \) is a union of path graphs \( P_2 \).

\textbf{Proof} Recall that we have for any function \( h \)

\[
\sum_{uv \in E(G)} (h(d_u) + h(d_v)) = \sum_{u \in V(G)} d_u h(d_u).
\]
In particular,
\[ \sum_{uv \in E(G)} (d_u^a + d_v^a) = \sum_{u \in V(G)} d_u^{a+1} = M_{1}^{a+1}(G). \]

The function \( f(x) = x + 1/x \) is strictly decreasing on \((0, 1]\) and strictly increasing on \([1, \infty)\), and so, \( f(x) \geq f(1) = 2 \) for every \( x > 0 \). Hence,
\[
\frac{1}{d_u^a + d_v^a} + d_u^a + d_v^a \geq 2, \\
ISD_a(G) + M_1^{a+1}(G) \geq 2m.
\]

If \( a > 0 \), then \( d_u^a + d_v^a \geq 2 \) and
\[
\frac{1}{d_u^a + d_v^a} + d_u^a + d_v^a \geq f(2) = \frac{5}{2}, \\
ISD_a(G) + M_1^{a+1}(G) \geq \frac{5}{2}m.
\]

The previous argument gives that the equality in this bound is attained if and only if \( d_u = d_v = 1 \) for every \( uv \in E(G) \), i.e., \( G \) is a union of path graphs \( P_2 \).

**Theorem 7** Let \( G \) be a graph with minimum degree \( \delta \) and \( m \) edges, and \( a \in \mathbb{R} \).

1. If \( a > 0 \), then
\[
ISD_a(G) + M_1^{a+1}(G) \geq \left(2\delta^a + \frac{1}{2\delta^a}\right)m.
\]

2. If \( \delta > 1 \) and \( a \leq -\log 2/\log \delta \), then
\[
ISD_a(G) + M_1^{a+1}(G) \geq \left(2\delta^a + \frac{1}{2\delta^a}\right)m.
\]

The equality in each bound is attained if and only if \( G \) is regular.

**Proof** If \( a > 0 \), then \( d_u^a + d_v^a \geq 2\delta^a \geq 2 > 1 \). The argument in the proof of Theorem 6 gives
\[
\frac{1}{d_u^a + d_v^a} + d_u^a + d_v^a \geq f(2\delta^a) = 2\delta^a + \frac{1}{2\delta^a}, \\
ISD_a(G) + M_1^{a+1}(G) \geq \left(2\delta^a + \frac{1}{2\delta^a}\right)m.
\]

If \( \delta > 1 \) and \( a \leq -\log 2/\log \delta < 0 \), then \( 2\delta^a \leq 1 \) and \( d_u^a + d_v^a \leq 2\delta^a \leq 1 \).

Thus,
\[
\frac{1}{d_u^a + d_v^a} + d_u^a + d_v^a \geq f(2\delta^a) = 2\delta^a + \frac{1}{2\delta^a}, \\
ISD_a(G) + M_1^{a+1}(G) \geq \left(2\delta^a + \frac{1}{2\delta^a}\right)m.
\]

The previous argument gives that the equality in each bound is attained if and only if \( d_u^a + d_v^a = 2\delta^a \) for every \( uv \in E(G) \), i.e., \( d_u = d_v = \delta \) for every \( uv \in E(G) \); and this holds if and only if \( G \) is regular.
Theorem 8 Let $G$ be a graph with maximum degree $\Delta$ and $m$ edges, and $a > 0$. Then

$$ISD_a(G) + M_1^{a+1}(G) \leq \left(2\Delta^a + \frac{1}{2\Delta^a}\right)m,$$

and the equality in the bound is attained if and only if $G$ is regular.

Proof If $a > 0$, then $1 < 2 \leq d_u^a + d_v^a \leq 2\Delta^a$. The argument in the proof of Theorem 6 gives

$$\frac{1}{d_u^a + d_v^a} + \frac{1}{2\Delta^a} \leq f(2\Delta^a) = 2\Delta^a + \frac{1}{2\Delta^a}.$$

The previous argument gives that the equality in the bound is attained if and only if $d_u^a + d_v^a = 2\Delta^a$ for every $uv \in E(G)$, i.e., $d_u = d_v = \Delta$ for every $uv \in E(G)$; and this holds if and only if $G$ is regular.

We need the following well known result, that provides a converse of the Cauchy-Schwarz inequality (see, e.g., [19, Lemma 3.4]).

Lemma 1 If $a_j, b_j \geq 0$ and $\omega b_j \leq a_j \leq \Omega b_j$ for $1 \leq j \leq k$, then

$$\left(\sum_{j=1}^k a_j^2\right)^{1/2} \left(\sum_{j=1}^k b_j^2\right)^{1/2} \leq \frac{1}{2} \left(\sqrt{\frac{\Omega}{\omega}} + \sqrt{\frac{\omega}{\Omega}}\right) \sum_{j=1}^k a_j b_j.$$

If $a_j > 0$ for some $1 \leq j \leq k$, then the equality holds if and only if $\omega = \Omega$ and $a_j = \omega b_j$ for every $1 \leq j \leq k$.

Recall that a $(\Delta, \delta)$-biregular graph is a bipartite graph for which any vertex in one side of the given bipartition has degree $\Delta$ and any vertex in the other side of the bipartition has degree $\delta$.

Theorem 9 If $G$ is a graph with $m$ edges, maximum degree $\Delta$ and minimum degree $\delta$, and $a \in \mathbb{R} \setminus \{0\}$, then

$$m^2 \leq ISD_a(G)M_1^{a+1}(G) \leq \frac{(\Delta^a + \delta^a)^2}{4\Delta^a\delta^a} m^2.$$  (6)

The equality in the upper bound is attained if and only if $G$ is regular. The equality in the lower bound is attained if $G$ is regular or biregular. Furthermore, if $G$ is a connected graph, then the equality in the lower bound is attained if and only if $G$ is a regular or biregular graph.

Proof Cauchy-Schwarz inequality gives

$$m^2 = \left(\sum_{uv \in E(G)} \frac{1}{d_u^a + d_v^a} \sqrt{d_u^2 + d_v^2}\right)^2 \leq \sum_{uv \in E(G)} \frac{1}{d_u^a + d_v^a} \sum_{uv \in E(G)} (d_u^a + d_v^a) = ISD_a(G)M_1^{a+1}(G).$$
If $a > 0$, then
\[ 2\delta^a \leq d_u^a + d_v^a = \frac{\sqrt{d_u^a + d_v^a}}{\sqrt{d_u^a + d_v^a}} \leq 2\Delta^a. \]

If $a < 0$, then
\[ 2\Delta^a \leq d_u^a + d_v^a = \frac{\sqrt{d_u^a + d_v^a}}{\sqrt{d_u^a + d_v^a}} \leq 2\delta^a. \]

Lemma 1 gives for every $a \neq 0$
\[ m^2 = \left( \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u^a + d_v^a}} \right)^2 \geq \sum_{uv \in E(G)} \frac{1}{d_u^a + d_v^a} \sum_{uv \in E(G)} \left( d_u^a + d_v^a \right) \frac{1}{\left( \frac{d_u^a + d_v^a}{d_u^a + d_v^a} \right)^2} = \frac{4\Delta^a \delta^a}{(\Delta^a + \delta^a)^2} ISD_a(G) M^{a+1}_1(G). \]

If $G$ is a regular graph, then the lower and upper bounds are the same, and they are equal to $ISD_a(G) M^{a+1}_1(G)$.

Assume now that the equality in the upper bound is attained. Lemma 1 gives $2\Delta^a = 2\delta^a$ and so, $\Delta = \delta$ and $G$ is regular.

If $G$ is a regular or biregular graph, then
\[ ISD_a(G) M^{a+1}_1(G) = \frac{m}{\Delta^a + \delta^a} (\Delta^a + \delta^a) m = m^2, \quad (7) \]
and the lower bound is attained.

Assume now that $G$ is a connected graph. By Cauchy-Schwarz inequality, the equality in the lower bound is attained if only if there exists a constant $\eta$ such that, for every $uv \in E(G)$,
\[ \frac{1}{\sqrt{d_u^a + d_v^a}} = \eta \sqrt{d_u^a + d_v^a}, \quad d_u^a + d_v^a = \eta^{-1}. \quad (8) \]

If $uv, uw \in E(G)$, then
\[ \eta^{-1} = d_u^a + d_w^a = d_u^a + d_w^a, \]
and $d_w = d_v$, since $h(t) = t^a$ is a one to one function. Thus, we conclude that $\eta$ is equivalent to the following: for each vertex $u \in V(G)$, every neighbor of $u$ has the same degree. Since $G$ is connected, this holds if and only if $G$ is regular or biregular.
3 Computational study of the ISD$_a$ index on random graphs

Here we follow a recently introduced approach under which topological indices are applied to ensembles of random graphs. Thus instead of computing the index of a single graph, the index average value over a large number of random graphs is measured as a function of the random graph parameters; see the application of this approach to Erdős-Rényi graphs and random regular graphs in [16,2,1,17].

We consider random graphs $G$ from the standard Erdős-Rényi (ER) model $G(n, p)$, i.e., $G$ has $n$ vertices and each edge appears independently with probability $p \in (0, 1)$. The computational study of the ISD$_a$ index we perform below is justified by the random nature of the ER model: since a given parameter pair $(n, p)$ represents an infinite-size ensemble of ER graphs, the computation of a ISD$_a$ index on a single ER graph is irrelevant. In contrast, the computation of $\langle \text{ISD}_a \rangle$ over a large ensemble of ER graphs, all characterized by the same parameter pair $(n, p)$, may provide useful average information about the ensemble. Also, we extend some of the inequalities derived in the previous Section to index average values.

3.1 Scaling of the average ISD$_a$ index on random graphs

In Fig. 1(a) we plot the average variable inverse sum deg index $\langle \text{ISD}_a(G) \rangle$ as a function of the probability $p$ of ER graphs of size $n = 1000$. There, we show curves for $a \in [-2, 2]$. As a reference we plot in different colors the curves corresponding to $a = -1$ (blue), $a = 0$ (red), and $a = 1$ (green). Recall that $\text{ISD}_{-1}(G) = \text{ISI}(G)$ and $\text{ISD}_1(G) = \chi(G)$. While for $a = 0$, $\langle \text{ISD}_0(G) \rangle$ gives half of the average number of edges of the ER graph; that is,

$$\langle \text{ISD}_0(G) \rangle = \sum_{uv \in E(G)} \frac{1}{d_u + d_v} = \frac{1}{2} |E(G)| = \frac{1}{4} n(n - 1)p .$$

(9)

Also, from Fig. 1(a) we observe that the curves of $\langle \text{ISD}_a(G) \rangle$ show three different behaviors as a function of $p$ depending on the value of $a$: For $a < a_0$, they grow for small $p$, approach a maximum value and then decrease when $p$ is further increased. For $a > a_0$, they are monotonically increasing functions of $p$. For $a = a_0$ the curves saturate above a given value of $p$. Here $a_0 = 1$.

Moreover, when $np \gg 1$, we can write $d_u \approx d_v \approx \langle d \rangle$, with

$$\langle d \rangle \approx (n - 1)p .$$

(10)

Therefore, for $np \gg 1$, $\langle \text{ISD}_a(G) \rangle$ is well approximated by:

$$\langle \text{ISD}_a(G) \rangle \approx \sum_{uv \in E(G)} \frac{1}{(d_u + d_v)^a} = |E(G)| \frac{1}{2} \langle d \rangle^a \approx \frac{n}{4} [(n - 1)p]^{1-a} .$$

(11)

In Fig. 1(b), we show that Eq. (11) (red-dashed lines) indeed describes well the data (thick black curves) for $np \geq 10$. 
Fig. 1  (a,b) Average variable inverse sum deg index $\langle ISD_{\alpha}(G) \rangle$ as a function of the probability $p$ of Erdős-Rényi graphs of size $n = 1000$. Here we show curves for $\alpha \in [-2, 2]$ in steps of 0.2 (from top to bottom). Blue, red and green curves in (a) correspond to $\alpha = -1$, $\alpha = 0$ and $\alpha = 1$, respectively. The red dashed lines in (b) are Eq. (11). The blue dashed line in (b) marks $\langle d \rangle = 10$. (c) $\langle ISD_{\alpha}(G) \rangle$ as a function of the probability $p$ of ER graphs of four different sizes $n$. (d) $\langle ISD_{\alpha}(G) \rangle / n$ as a function of the average degree $\langle d \rangle$. Same curves as in panel (c). The inset in (d) is the enlargement of the cyan rectangle. All averages are computed over $10^7/n$ random graphs.

Now in Fig. 1(c) we show $\langle ISD_{\alpha}(G) \rangle$ as a function of the probability $p$ of ER random graphs of four different sizes $n$. It is quite clear from this figure that the blocks of curves, characterized by the different graph sizes, display similar curves but displaced on both axes. Thus, our next goal is to find the scaling parameters that make the blocks of curves to coincide.

First, we recall that the average degree $\langle d \rangle$, see Eq. (10), is known to scale both topological and spectral measures applied to ER graphs. In particular, $\langle d \rangle$ was shown to scale the normalized Randic index [16], the normalized Harmonic [17] index, as well as several variable degree–based indices [1] on ER graphs. Thus, we expect $\langle ISD_{\alpha}(G) \rangle \propto f(\langle d \rangle)$. Second, we observe in Fig. 1(c) that the effect of increasing the graph size is to displace the blocks of curves $\langle ISD_{\alpha}(G) \rangle$ vs. $p$, characterized by the different graph sizes, upwards in the $y$–axis. Moreover, the fact that these blocks of curves, plotted in semi-log scale, are shifted the same amount on the $y$–axis when doubling $n$ is a clear signature of scalings of the form $\langle ISD_{\alpha}(G) \rangle \propto n^\beta$. By plotting $\langle ISD_{\alpha}(G) \rangle$ vs. $n$ for given values of $p$ (not shown here) we conclude that $\beta = 1$ for all $\alpha$. 
Therefore, in Fig. 1(d) we plot $\langle ISD_a(G) \rangle/n$ as a function of $\langle d \rangle$ showing that all curves are now properly scaled; i.e. the blocks of curves painted in different colors for different graph sizes fall on top of each other (see a detailed view in the inset of this figure). Moreover, following Eq. (11), we obtain

$$\frac{\langle ISD_a(G) \rangle}{n} \approx \frac{1}{4} \langle d \rangle^{1-a}. \quad (12)$$

We have verified that Eq. (12) is valid when $\langle d \rangle \geq 10$.

3.2 Inequalities of the average $ISD_a$ index on random graphs

Most inequalities obtained in the previous Section are not restricted to any particular type of graph. Thus, they should also be valid for random graphs and, moreover, can be extended to index average values, as needed in computational studies of random graphs.

Now, in order to ease the computational validation of some of the inequalities derived in the previous Section, we:

(i) write the right inequality of Eq. (1) in Theorem 3 as

$$0 \leq \langle 2^{a-1} \chi_a(G) - ISD_a(G) \rangle, \quad \text{if } a > 1, \quad (13)$$

(ii) write the left inequality of Eq. (2) in Theorem 3 as

$$0 \leq \langle ISD_a(G) - 2^{a-1} \chi_a(G) \rangle, \quad \text{if } 0 < a < 1, \quad (14)$$

(iii) write the inequality of Eq. (3) in Theorem 3 as

$$0 \leq \langle 2^{a-1} \chi_a(G) - ISD_a(G) \rangle, \quad \text{if } a < 0, \quad (15)$$

(iv) write the inequality of Eq. (4) in Theorem 6 as

$$\frac{5}{2} \langle m \rangle \leq \langle ISD_a(G) + M_1^{a+1}(G) \rangle, \quad \text{if } a > 0, \quad (16)$$

(v) write the inequality of Eq. (5) in Theorem 6 as

$$2 \langle m \rangle \leq \langle ISD_a(G) + M_1^{a+1}(G) \rangle, \quad \text{if } a < 0, \quad (17)$$

and

(vi) write the left inequality of Eq. (6) in Theorem 9 as

$$\langle m^2 \rangle \leq \langle ISD_a(G) M_1^{a+1}(G) \rangle. \quad (18)$$

Therefore, in Figs. 2(a-f) we plot the r.h.s. of the inequalities (13-18), respectively, as a function of the probability $p$ of ER graphs of size $n = 100$.

In particular, since the curves in Figs. 2(a-c) are all positive, the inequalities (13-15) are easily validated. Now, in order validate inequalities (16,17) we include (as dashed lines) in both Fig. 2(d) and Fig. 2(e) the functions $(5/2) \langle m \rangle$ vs. $p$ (red) and $2 \langle m \rangle$ vs. $p$ (blue); where we used $\langle m \rangle = n(n-1)p/2$. Then,
we can clearly see that all curves $\langle ISD_a(G) + M_{a+1}^1(G) \rangle$ vs. $p$ in Fig. 2(d) lie above the red dashed line, corresponding to $(5/2)\langle m \rangle$; while all curves $\langle ISD_a(G) + M_{a+1}^1(G) \rangle$ vs. $p$ in Fig. 2(e) lie above the blue dot-dashed line, corresponding to $2\langle m \rangle$. This can be better appreciated in the enlargements shown in the panel insets. Finally, in Fig. 2(f) we include, as a red dashed line, the function $\langle m^2 \rangle$ vs. $p$ to clearly show that all curves $\langle ISD_a(G)M_{a+1}^1(G) \rangle$ vs. $p$ lie above it, as stated in inequality (18). Moreover, note that the equality in (18) is attained for $p \to 1$. This is indeed expected since for $np \gg 1$ we can...
write
\[
\langle ISD_a(G)M_1^{a+1}(G) \rangle = \left\langle \sum_{uv \in E(G)} \frac{1}{d_u^a + d_v^a} \sum_{uv \in E(G)} d_u^a + d_v^a \right\rangle \\
\approx \left\langle \sum_{uv \in E(G)} \frac{1}{\langle d \rangle^a + \langle d \rangle^a} \sum_{uv \in E(G)} \langle d \rangle^a + \langle d \rangle^a \right\rangle \\
= \left\langle \frac{m}{\langle d \rangle^a + \langle d \rangle^a}m\langle d \rangle^a + \langle d \rangle^a \right\rangle = \langle m^2 \rangle ,
\]
which we have observed to be valid for several graph sizes when \( \langle d \rangle \geq 10 \).

4 Summary

In this work we performed analytical and computational studies of the variable inverse sum deg index \( ISD_a(G) \). First, we analytically obtained new inequalities connecting \( ISD_a(G) \) with other well-known topological indices such as the Randić index, the general sum-connectivity index, the geometric-arithmetic index, the arithmetic-geometric index, as well as the variable first Zagreb index. Then, we computationally validated some of the obtained inequalities on ensembles of Erdős-Rényi graphs \( G(n, p) \) characterized by \( n \) vertices connected independently with probability \( p \in (0, 1) \). Additionally, we showed that the ratio \( \langle ISD_a(G) \rangle / n \) depends only on the average degree \( \langle d \rangle = (n - 1)p \).

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Conflict of interest

The authors declare that they have no conflict of interest.

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