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Research article

Analytical and computational properties of the variable symmetric division deg index

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Abstract: The aim of this work is to obtain new inequalities for the variable symmetric division deg index $SDD_\alpha(G) = \sum_{uv\in E(G)}(d_u^\alpha/d_v^\alpha + d_v^\alpha/d_u^\alpha)$, and to characterize graphs extremal with respect to them. Here, by uv we mean the edge of a graph G joining the vertices u and v, and d_u denotes the degree of u, and $\alpha \in \mathbb{R}$. Some of these inequalities generalize and improve previous results for the symmetric division deg index. In addition, we computationally apply the $SDD_\alpha(G)$ index on random graphs and we demonstrate that the ratio $\langle SDD_\alpha(G)\rangle /n$ (n is the order of the graph) depends only on the average degree $\langle d\rangle$.

Keywords: symmetric division deg index; degree-based topological index; random graphs

1. Preliminaries

By a graph $G = (V(G), E(G))$, with $V(G)$ and $E(G)$ the set of vertices and edges of G respectively, we mean an undirected simple graph without isolated vertices (i.e., each vertex has at least a neighbor).

Given a graph G, representing a chemical structure,

$$X(G) = \sum_{uv\in E(G)} F(d_u, d_v)$$

is said a topological descriptor and, if also it correlates with a molecular property, it is called a topological index. Above, by uv we mean the edge of a graph G joining the vertices u and v, d_u denotes the degree of u, and F is an appropriate chosen function. Remarkably, topological indices capture physical properties of a chemical compound in a single number.

A great number of topological indices have been defined and studied over more than four decades. Among them, probably the most popular topological indices are the Randić and the Zagreb indices. The first and second Zagreb indices, denoted by M_1 and M_2, respectively, were defined by Gutman and Trinajstić (see [1]) in 1972 by

$$M_1(G) = \sum_{u\in V(G)} d_u^2, \qquad M_2(G) = \sum_{uv\in E(G)} d_u d_v.$$

For more details of the applications and mathematical properties of Zagreb indices see [2–4], and the references therein. Zagreb indices have many connections with other topological indices, see e.g., [5,6].

The concept of variable molecular descriptors was proposed as a way of characterizing heteroatoms (see [7, 8]), but also to assess structural differences in alkylcycloalkanes [9]. The idea behind the variable molecular descriptors is that the variables are determined during the regression in order to minimize the error of estimate for a particular chemical property (see, e.g., [10]).

In this line of ideas, the variable versions of the first and second Zagreb indices were introduced as [10–12]

$$M_1^{\alpha}(G) = \sum_{u\in V(G)} d_u^{\alpha}, \qquad M_2^{\alpha}(G) = \sum_{uv\in E(G)} (d_u d_v)^{\alpha},$$

with $\alpha \in \mathbb{R}$. Evidently, M_1^2 and M_2^1 are the first and second Zagreb indices, respectively. In addition, *the first and second variable Zagreb indices* include several known indices. As examples we note that $M_2^{-1/2}$ is the Randić index, M_1^3 is the forgotten index F, M_1^{-1} is the inverse index ID, and M_2^{-1} is the modified Zagreb index.

In 2011, Vukičević proposed the *variable symmetric division deg index* [13]

$$SDD_{\alpha}(G) = \sum_{uv\in E(G)} \left(\frac{d_u^{\alpha}}{d_v^{\alpha}} + \frac{d_v^{\alpha}}{d_u^{\alpha}} \right). \tag{1.1}$$

Note that $SDD_{-\alpha}(G) = SDD_{\alpha}(G)$ and so, it suffices to consider positive values of α. The symmetric division deg index is the best predictor of total surface area for polychlorobiphenyls [14].

In this work we perform studies of the variable symmetric division deg index from analytical and computational viewpoints. We obtain new inequalities for the variable symmetric division deg index $SDD_{\alpha}(G)$ and we characterize graphs extremal with respect to them. Some of these inequalities generalize and improve previous results for the symmetric division deg index. In addition, we computationally apply the $SDD_{\alpha}(G)$ index on random graphs and we demonstrate that the ratio $\langle SDD_{\alpha}(G)\rangle /n$ (n denotes the order of the graph) depends only on the average degree $\langle d\rangle$.

One of our main results is Theorem 8, which provides upper and lower bounds of $SDD_{\alpha}(G)$ in terms of the number of edges, the maximum and the minimum degree of G.

2. Analytical study of the variable symmetric division deg index

Let us start by proving a monotonicity property of these indices.

Theorem 1. *Let G be a graph and $0 < \alpha < \beta$. Then*

$$SDD_\alpha(G) \le SDD_\beta(G),$$

and the equality in the bound is attained if and only if each connected component of G is a regular graph.

Proof. Let us consider $x \ge 1$. Thus, $x^\alpha \ge x^{-\beta}$ and

$$x^{\beta-\alpha} - 1 \ge 0, \qquad x^\alpha(x^{\beta-\alpha} - 1) \ge x^{-\beta}(x^{\beta-\alpha} - 1),$$
$$x^\beta - x^\alpha \ge x^{-\alpha} - x^{-\beta}, \qquad x^\beta + x^{-\beta} \ge x^\alpha + x^{-\alpha},$$

for every $x \ge 1$. Since $u(x) = x^\alpha + x^{-\alpha}$ satisfies $u(1/x) = u(x)$ for every $x > 0$, we have $x^\beta + x^{-\beta} \ge x^\alpha + x^{-\alpha}$ for every $x > 0$. Note that we obtain the equality if and only if $x = 1$.

Thus, we have

$$SDD_\beta(G) = \sum_{uv\in E(G)} \left(\frac{d_u^\beta}{d_v^\beta} + \frac{d_v^\beta}{d_u^\beta} \right) \ge \sum_{uv\in E(G)} \left(\frac{d_u^\alpha}{d_v^\alpha} + \frac{d_v^\alpha}{d_u^\alpha} \right) = SDD_\alpha(G).$$

The previous argument gives that we have the equality in the bound if and only if $d_u/d_v = 1$ for every $uv \in E(G)$, i.e., each connected component of G is a regular graph.

Our next results in this section provide bounds of $SDD_\alpha(G)$ involving the maximum and minimum degree of the graph G. Since scientists often estimate average degree of large networks, we present in the next section results involving the average degree.

Our next theorem relates the SDD_α and the variable Zagreb indices.

Theorem 2. *If G is a graph with minimum degree δ and maximum degree Δ, and $\alpha > 0$, then*

$$2\delta^{2\alpha} M_2^{-\alpha}(G) \le SDD_\alpha(G) \le 2\Delta^{2\alpha} M_2^{-\alpha}(G),$$
$$\Delta^{-2\alpha} M_1^{2\alpha+1}(G) \le SDD_\alpha(G) \le \delta^{-2\alpha} M_1^{2\alpha+1}(G),$$

and we have the equality in each bound if and only if G is regular.

Proof. First of all recall that for every function f the following equality

$$\sum_{uv\in E(G)} (f(d_u) + f(d_v)) = \sum_{u\in V(G)} d_u f(d_u)$$

holds. In particular,

$$\sum_{uv\in E(G)} (d_u^{2\alpha} + d_v^{2\alpha}) = \sum_{u\in V(G)} d_u^{2\alpha+1} = M_1^{2a+1}(G).$$

Since

$$SDD_\alpha(G) = \sum_{uv\in E(G)} \left(\frac{d_u^\alpha}{d_v^\alpha} + \frac{d_v^\alpha}{d_u^\alpha} \right) = \sum_{uv\in E(G)} \frac{d_u^{2\alpha} + d_v^{2\alpha}}{(d_u d_v)^\alpha}.$$

and $\alpha > 0$, we obtain

$$SDD_\alpha(G) = \sum_{uv\in E(G)} \frac{d_u^{2\alpha} + d_v^{2\alpha}}{(d_u d_v)^\alpha} \le 2\Delta^{2\alpha} \sum_{uv\in E(G)} (d_u d_v)^{-\alpha} = 2\Delta^{2\alpha} M_2^{-\alpha}(G),$$

and

$$SDD_\alpha(G) = \sum_{uv\in E(G)} \frac{d_u^{2\alpha} + d_v^{2\alpha}}{(d_u d_v)^\alpha} \geq 2\delta^{2\alpha} \sum_{uv\in E(G)} (d_u d_v)^{-\alpha} = 2\delta^{2\alpha} M_2^{-\alpha}(G).$$

We also have

$$\begin{aligned} SDD_\alpha(G) &= \sum_{uv\in E(G)} \frac{d_u^{2\alpha} + d_v^{2\alpha}}{(d_u d_v)^\alpha} \leq \delta^{-2\alpha} \sum_{uv\in E(G)} (d_u^{2\alpha} + d_v^{2\alpha}) \\ &= \delta^{-2\alpha} \sum_{u\in V(G)} d_u^{2\alpha+1} = \delta^{-2\alpha} M_1^{2\alpha+1}(G), \end{aligned}$$

and

$$\begin{aligned} SDD_\alpha(G) &= \sum_{uv\in E(G)} \frac{d_u^{2\alpha} + d_v^{2\alpha}}{(d_u d_v)^\alpha} \geq \Delta^{-2\alpha} \sum_{uv\in E(G)} (d_u^{2\alpha} + d_v^{2\alpha}) \\ &= \Delta^{-2\alpha} \sum_{u\in V(G)} d_u^{2\alpha+1} = \Delta^{-2\alpha} M_1^{2\alpha+1}(G). \end{aligned}$$

If G is a regular graph, then each lower bound and its corresponding upper bound are the same, and both are equal to $SDD_\alpha(G)$.

Assume now that the equality in either the first or second bound holds. The previous argument gives that we have either $d_u^{2\alpha} + d_v^{2\alpha} = 2\Delta^{2\alpha}$ for any $uv \in E(G)$ or $d_u^{2\alpha} + d_v^{2\alpha} = 2\delta^{2\alpha}$ for any $uv \in E(G)$. Since $\alpha > 0$, we have $\delta^{2\alpha} \leq d_u^{2\alpha}, d_v^{2\alpha} \leq \Delta^{2\alpha}$, and we conclude that $d_u = d_v = \Delta$ for any $uv \in E(G)$, or $d_u = d_v = \delta$ for any $uv \in E(G)$. Hence, G is a regular graph.

Finally, assume that the equality in either the third or fourth bound holds. The previous argument gives that we have either $(d_u d_v)^\alpha = \delta^{2\alpha}$ for any $uv \in E(G)$ or $(d_u d_v)^\alpha = \Delta^{2\alpha}$ for any $uv \in E(G)$. Since $\alpha > 0$, we have $\delta^\alpha \leq d_u^\alpha, d_v^\alpha \leq \Delta^\alpha$, and we conclude that $d_u = d_v = \delta$ for any $uv \in E(G)$, or $d_u = d_v = \Delta$ for every $uv \in E(G)$. Therefore, G is a regular graph.

We will need the following technical result.

Lemma 3. *Let* $0 < a < A$. *Then*

$$a \leq \frac{x^2 + y^2}{x + y} \leq A$$

for every $a \leq x, y \leq A$. *The lower bound is attained if and only if* $x = y = a$. *The upper bound is attained if and only if* $x = y = A$.

Proof. If $a \leq x, y \leq A$, then $ax + ay \leq x^2 + y^2 \leq Ax + Ay$, and the statement holds.

A large kind of topological indices, named *Adriatic indices*, was introduced in [14, 15]. Twenty of them were selected as significant predictors of chemical properties. One of them, the *inverse sum indeg* index, defined by

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

appears in [14, 15] as a good predictor of total surface area of octane isomers.

Next, we relate $SDD_\alpha(G)$ with 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.

Theorem 4. *If G is a graph with m edges and minimum degree δ, and $\alpha > 0$, then*

$$SDD_\alpha(G) \geq \frac{\delta^\alpha m^2}{ISD_{-\alpha}(G)},$$

and the equality in the bound holds if and only if G is regular.

Proof. Lemma 3 gives

$$\delta^\alpha \leq \frac{x^{2\alpha} + y^{2\alpha}}{x^\alpha + y^\alpha} \leq \Delta^\alpha, \qquad \frac{1}{x^{2\alpha} + y^{2\alpha}} \leq \frac{\delta^{-\alpha}}{x^\alpha + y^\alpha}, \qquad \frac{1}{d_u^{2\alpha} + d_v^{2\alpha}} \leq \frac{\delta^{-\alpha}}{d_u^\alpha + d_v^\alpha},$$

for every $\delta \leq x, y \leq \Delta$. This last inequality and Cauchy-Schwarz inequality give

$$\begin{aligned} m^2 &= \Big(\sum_{uv \in E(G)} 1 \Big)^2 = \Big(\sum_{uv \in E(G)} \Big(\frac{d_u^{2\alpha} + d_v^{2\alpha}}{d_u^\alpha d_v^\alpha} \Big)^{1/2} \Big(\frac{d_u^\alpha d_v^\alpha}{d_u^{2\alpha} + d_v^{2\alpha}} \Big)^{1/2} \Big)^2 \\ &\leq \sum_{uv \in E(G)} \frac{d_u^{2\alpha} + d_v^{2\alpha}}{d_u^\alpha d_v^\alpha} \sum_{uv \in E(G)} \frac{d_u^\alpha d_v^\alpha}{d_u^{2\alpha} + d_v^{2\alpha}} \\ &\leq \delta^{-\alpha} SDD_\alpha(G) \sum_{uv \in E(G)} \frac{d_u^\alpha d_v^\alpha}{d_u^\alpha + d_v^\alpha} \\ &= \delta^{-\alpha} SDD_\alpha(G) \sum_{uv \in E(G)} \frac{1}{d_u^{-\alpha} + d_v^{-\alpha}} \\ &= \delta^{-\alpha} SDD_\alpha(G)\, ISD_{-\alpha}(G). \end{aligned}$$

If G is a regular graph, then $SDD_\alpha(G) = 2m$, $ISD_{-\alpha}(G) = m\delta^\alpha/2$ and the equality in the bound holds.

Assume now that the equality in the bound holds. Thus, by the previous argument,

$$\frac{1}{d_u^{2\alpha} + d_v^{2\alpha}} = \frac{\delta^{-\alpha}}{d_u^\alpha + d_v^\alpha}$$

for any $uv \in E(G)$. Then Lemma 3 gives $d_u = d_v = \delta$ for any $uv \in E(G)$. Hence, G is a regular graph.

The *modified Narumi-Katayama index* is defined by

$$NK^*(G) = \prod_{u \in V(G)} d_u^{d_u} = \prod_{uv \in E(G)} d_u d_v$$

in [16], inspired in the Narumi-Katayama index [17]. Next, we present an inequality relating $SDD_\alpha(G)$ and $NK^*(G)$.

Theorem 5. *Let G be a graph with m edges and minimum degree δ, and $\alpha > 0$. Then*

$$SDD_\alpha(G) \geq 2\delta^{2\alpha} m NK^*(G)^{-\alpha/m},$$

and the equality in the bound holds if and only if G is a regular graph.

Proof. Since the geometric mean is at most the arithmetic mean, we have

$$\begin{aligned}\frac{1}{m}SDD_\alpha(G) &= \frac{1}{m}\sum_{uv\in E(G)}\left(\frac{d_u^\alpha}{d_v^\alpha}+\frac{d_v^\alpha}{d_u^\alpha}\right) = \frac{1}{m}\sum_{uv\in E(G)}\frac{d_u^{2\alpha}+d_v^{2\alpha}}{(d_ud_v)^\alpha}\\ &\ge 2\delta^{2\alpha}\frac{1}{m}\sum_{uv\in E(G)}\frac{1}{(d_ud_v)^\alpha} \ge 2\delta^{2\alpha}\left(\prod_{uv\in E(G)}\frac{1}{(d_ud_v)^\alpha}\right)^{1/m}\\ &= 2\delta^{2\alpha}NK^*(G)^{-\alpha/m}.\end{aligned}$$

If G is a regular graph, then

$$2\delta^{2\alpha}mNK^*(G)^{-\alpha/m} = 2\delta^{2\alpha}m(\delta^{2m})^{-\alpha/m} = 2m = SDD_\alpha(G).$$

Finally, assume that the equality in the bound holds. The previous argument gives that $d_u^{2\alpha}+d_v^{2\alpha} = 2\delta^{2\alpha}$ for any $uv \in E(G)$. Since $\alpha > 0$, we obtain $\delta^{2\alpha} \le d_u^{2\alpha}, d_v^{2\alpha}$, and we have $d_u = d_v = \delta$ for any $uv \in E(G)$. Hence, G is regular.

Next, we obtain additional bounds of SDD_α.

Theorem 6. *Let G be a graph with m edges, minimum degree δ and maximum degree $\delta+1$, $\alpha > 0$ and let A be the number of edges $uv \in E(G)$ with $d_u \neq d_v$. Then A is an even integer and*

$$SDD_\alpha(G) = 2m + A\left(\frac{(\delta+1)^\alpha}{\delta^\alpha}+\frac{\delta^\alpha}{(\delta+1)^\alpha}-2\right).$$

Proof. Let $F = \{uv \in E(G) : d_u \neq d_v\}$, then A is the cardinality of the set F. Since the maximum degree of G is $\delta+1$ and its minimum degree is δ, if $uv \in F$, then $d_u = \delta$ and $d_v = \delta+1$ or viceversa, and therefore

$$\frac{d_u^\alpha}{d_v^\alpha}+\frac{d_v^\alpha}{d_u^\alpha} = \frac{(\delta+1)^\alpha}{\delta^\alpha}+\frac{\delta^\alpha}{(\delta+1)^\alpha}.$$

If $uv \in F^c = E(G)\setminus F$, then $d_u = d_v = \delta$ or $d_u = d_v = \delta+1$, and therefore

$$\frac{d_u^\alpha}{d_v^\alpha}+\frac{d_v^\alpha}{d_u^\alpha} = 2.$$

Since there are exactly A edges in F and $m-A$ edges in F^c, we have

$$\begin{aligned}SDD_\alpha(G) &= \sum_{uv\in E(G)}\Big(\frac{d_u^\alpha}{d_v^\alpha}+\frac{d_v^\alpha}{d_u^\alpha}\Big)\\ &= \sum_{uv\in F^c}\Big(\frac{d_u^\alpha}{d_v^\alpha}+\frac{d_v^\alpha}{d_u^\alpha}\Big)+\sum_{uv\in F}\Big(\frac{d_u^\alpha}{d_v^\alpha}+\frac{d_v^\alpha}{d_u^\alpha}\Big)\\ &= \sum_{uv\in F^c}2+\sum_{uv\in F}\Big(\frac{(\delta+1)^\alpha}{\delta^\alpha}+\frac{\delta^\alpha}{(\delta+1)^\alpha}\Big)\\ &= 2m-2A+A\Big(\frac{(\delta+1)^\alpha}{\delta^\alpha}+\frac{\delta^\alpha}{(\delta+1)^\alpha}\Big).\end{aligned}$$

This gives the equality.

Seeking for a contradiction assume that A is an odd integer.

Let Γ_1 be a subgraph of G obtained as follows: Γ_1 is induced by the n_1 vertices with degree δ in $V(G)$; denote by m_1 the number of edges of Γ_1. Handshaking Lemma implies $n_1\delta - A = 2m_1$. Since A is an odd integer, δ is also an odd integer. Thus, $\delta + 1$ is even.

Let Γ_2 be the subgraph of G induced by the n_2 vertices with degree $\delta + 1$ in $V(G)$, and denote by m_2 the number of edges of Γ_2. Handshaking Lemma implies $n_2(\delta + 1) - A = 2m_2$, a contradiction, since A is odd and $\delta + 1$ is even.

Thus, we conclude that A is an even integer.

We will need the following result in the proof of Theorem 8 below.

Lemma 7. *Given $\alpha > 0$, consider the function $u : (0, \infty) \to (0, \infty)$ defined as $u(t) = t^{\alpha} + t^{-\alpha}$. Then u strictly decreases on $(0, 1]$, u strictly increases on $[1, \infty)$ and $u(t) \geq u(1) = 2$.*

Proof. We have

$$u'(t) = \alpha t^{\alpha-1} - \alpha t^{-\alpha-1} = \alpha t^{-\alpha-1}(t^{2\alpha} - 1).$$

Since $\alpha > 0$, we have $u' < 0$ on $(0, 1)$ and $u' > 0$ on $(1, \infty)$. This gives the result.

The following figure shows the function $u(t)$ for some values of α.

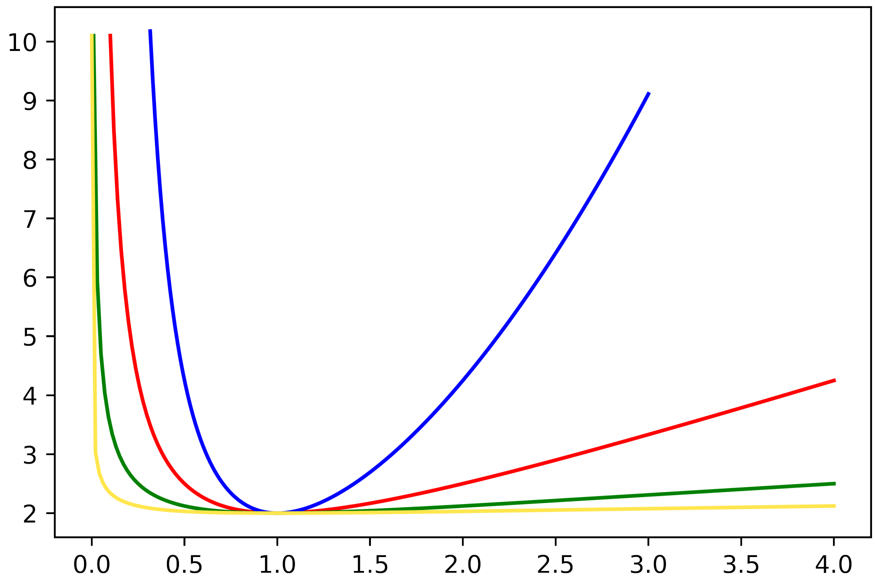

Figure 1. Representations of the function $u(t)$ of Lemma 7 for: $\alpha = 1/4$ (yellow), $\alpha = 1/2$ (green), $\alpha = 1$ (red) and $\alpha = 2$ (blue).

Theorem 6 gives the precise value of SDD_{α} when $\Delta = \delta + 1$. Theorem 8 below provides a lower bound when $\Delta > \delta + 1$.

Theorem 8. *Let G be a graph with m edges, minimum degree δ and maximum degree $\Delta > \delta + 1$. Denote by A_0, A_1, A_2, the cardinality of the subsets of edges $F_0 = \{uv \in E(G) : d_u = \delta, d_v = \Delta\}$,*

$F_1 = \{uv \in E(G) : d_u = \delta, \delta < d_v < \Delta\}$, $F_2 = \{uv \in E(G) : d_u = \Delta, \delta < d_v < \Delta\}$, respectively. If $\alpha > 0$, then

$$SDD_\alpha(G) \le (m - A_1 - A_2)\left(\frac{\Delta^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{\Delta^\alpha}\right) + A_1\left(\frac{(\Delta-1)^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{(\Delta-1)^\alpha}\right)$$
$$+ A_2\left(\frac{\Delta^\alpha}{(\delta+1)^\alpha} + \frac{(\delta+1)^\alpha}{\Delta^\alpha}\right),$$
$$SDD_\alpha(G) \ge 2m + A_0\left(\frac{\Delta^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{\Delta^\alpha} - 2\right) + A_1\left(\frac{(\delta+1)^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{(\delta+1)^\alpha} - 2\right)$$
$$+ A_2\left(\frac{\Delta^\alpha}{(\Delta-1)^\alpha} + \frac{(\Delta-1)^\alpha}{\Delta^\alpha} - 2\right).$$

Proof. Lemma 7 gives that the function

$$\frac{d_v^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{d_v^\alpha} = u\left(\frac{d_v}{\delta}\right)$$

is increasing in $d_v \in [\delta+1, \Delta-1]$ and so,

$$\frac{(\delta+1)^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{(\delta+1)^\alpha} \le \frac{d_v^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{d_v^\alpha} \le \frac{(\Delta-1)^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{(\Delta-1)^\alpha},$$

for every $uv \in F_1$.

In a similar way, Lemma 7 gives that the function

$$\frac{\Delta^\alpha}{d_v^\alpha} + \frac{d_v^\alpha}{\Delta^\alpha} = u\left(\frac{d_v}{\Delta}\right)$$

is decreasing in $d_v \in [\delta+1, \Delta-1]$ and so,

$$\frac{\Delta^\alpha}{(\Delta-1)^\alpha} + \frac{(\Delta-1)^\alpha}{\Delta^\alpha} \le \frac{\Delta^\alpha}{d_v^\alpha} + \frac{d_v^\alpha}{\Delta^\alpha} \le \frac{\Delta^\alpha}{(\delta+1)^\alpha} + \frac{(\delta+1)^\alpha}{\Delta^\alpha},$$

for every $uv \in F_2$.

Also,

$$2 \le \frac{d_u^\alpha}{d_v^\alpha} + \frac{d_v^\alpha}{d_u^\alpha} \le \frac{\Delta^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{\Delta^\alpha}$$

for any $uv \in E(G)$.

We obtain

$$SDD_\alpha(G) = \sum_{uv \in E(G)\setminus(F_0\cup F_1\cup F_2)} \left(\frac{d_u^\alpha}{d_v^\alpha} + \frac{d_v^\alpha}{d_u^\alpha}\right) + \sum_{uv\in F_0}\left(\frac{d_u^\alpha}{d_v^\alpha} + \frac{d_v^\alpha}{d_u^\alpha}\right)$$
$$+ \sum_{uv\in F_1}\left(\frac{d_u^\alpha}{d_v^\alpha} + \frac{d_v^\alpha}{d_u^\alpha}\right) + \sum_{uv\in F_2}\left(\frac{d_u^\alpha}{d_v^\alpha} + \frac{d_v^\alpha}{d_u^\alpha}\right)$$
$$\ge \sum_{uv \in E(G)\setminus(F_0\cup F_1\cup F_2)} 2 + \sum_{uv\in F_0}\left(\frac{\Delta^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{\Delta^\alpha}\right)$$
$$+ \sum_{uv\in F_1}\left(\frac{d_v^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{d_v^\alpha}\right) + \sum_{uv\in F_2}\left(\frac{\Delta^\alpha}{d_v^\alpha} + \frac{d_v^\alpha}{\Delta^\alpha}\right).$$

Hence,

$$SDD_\alpha(G) \geq 2m - 2A_0 - 2A_1 - 2A_2 + A_0\left(\frac{\Delta^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{\Delta^\alpha}\right)$$
$$+ A_1\left(\frac{(\delta+1)^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{(\delta+1)^\alpha}\right) + A_2\left(\frac{\Delta^\alpha}{(\Delta-1)^\alpha} + \frac{(\Delta-1)^\alpha}{\Delta^\alpha}\right).$$

We also have

$$\begin{aligned} SDD_\alpha(G) &= \sum_{uv\in E(G)\setminus(F_1\cup F_2)}\left(\frac{d_u^\alpha}{d_v^\alpha} + \frac{d_v^\alpha}{d_u^\alpha}\right) \\ &\quad + \sum_{uv\in F_1}\left(\frac{d_u^\alpha}{d_v^\alpha} + \frac{d_v^\alpha}{d_u^\alpha}\right) + \sum_{uv\in F_2}\left(\frac{d_u^\alpha}{d_v^\alpha} + \frac{d_v^\alpha}{d_u^\alpha}\right) \\ &\leq (m - A_1 - A_2)\left(\frac{\Delta^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{\Delta^\alpha}\right) \\ &\quad + A_1\left(\frac{(\Delta-1)^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{(\Delta-1)^\alpha}\right) + A_2\left(\frac{\Delta^\alpha}{(\delta+1)^\alpha} + \frac{(\delta+1)^\alpha}{\Delta^\alpha}\right). \end{aligned}$$

3. Computational study of the variable symmetric division deg index on random graphs

Here we deal with two classes of random graphs G: Erdös-Rényi (ER) graphs $G(n, p)$ and bipartite random (BR) graphs $G(n_1, n_2, p)$. ER graphs are formed by n vertices connected independently with probability $p \in [0, 1]$. While BR graphs are composed by two disjoint sets, sets 1 and 2, with n_1 and n_2 vertices each such that there are no adjacent vertices within the same set, being $n = n_1 + n_2$ the total number of vertices in the bipartite graph. The vertices of the two sets are connected randomly with probability $p \in [0, 1]$. Another work in this spirit is [18].

We stress that the computational study of the variable symmetric division deg index we perform below is justified by the random nature of the graph models we want to explore. Since a given parameter set (n, p) $[(n_1, n_2, p)]$ represents an infinite-size ensemble of ER graphs [BR graphs], the computation of $SDD_\alpha(G)$ on a single graph is irrelevant. In contrast, the computation of $\langle SDD_\alpha(G)\rangle$ (where $\langle\cdot\rangle$ indicates ensemble average) over a large number of random graphs, all characterized by the same parameter set (n, p) $[(n_1, n_2, p)]$, may provide useful *average* information about the full ensemble. This *computational* approach, well known in random matrix theory studies, is not widespread in studies involving topological indices, mainly because topological indices are not commonly applied to random graphs; for very recent exceptions see [19–22].

3.1. Average properties of the SDD_α index on Erdös-Rényi random graphs

From the definition of the variable symmetric division deg index, see Eq (1.1), we have that:

(i) For $\alpha = 0$, $\langle SDD_0(G)\rangle$ gives twice the average number of edges of the ER graph. That is,

$$\begin{aligned} \langle SDD_0(G)\rangle &= \left\langle \sum_{uv\in E(G)}\left(\frac{d_u^0}{d_v^0} + \frac{d_v^0}{d_u^0}\right)\right\rangle = \left\langle \sum_{uv\in E(G)}(1+1)\right\rangle \\ &= \langle 2|E(G)|\rangle = n(n-1)p\,. \end{aligned} \tag{3.1}$$

(ii) When $np \gg 1$, we can approximate $d_u \approx d_v \approx \langle d \rangle$, then

$$\begin{aligned}\langle SDD_\alpha(G)\rangle &\approx \left\langle \sum_{uv\in E(G)} (1^\alpha + 1^\alpha) \right\rangle = \left\langle \sum_{uv\in E(G)} 2 \right\rangle \\ &= \langle 2|E(G)|\rangle = n(n-1)p\,. \end{aligned} \tag{3.2}$$

(iii) By recognizing that the average degree of the ER graph model reads as

$$\langle d \rangle = (n-1)p\,, \tag{3.3}$$

we can rewrite Eq (3.2) as

$$\frac{\langle SDD_\alpha(G)\rangle}{n} \approx \langle d \rangle\ . \tag{3.4}$$

We stress that Eq (3.4) is expected to be valid for $np \gg 1$.

In Figure 2(a) we plot $\langle SDD_\alpha(G)\rangle$ as a function of the probability p of ER graphs of size $n = 500$. All averages in Figure 2 are computed over ensembles of $10^7/n$ random graphs. In Figure 2(a) we show curves for $\alpha \in [0, 4]$. The dashed-magenta curve corresponds to the case $\alpha = 0$, which coincides with Eq (3.1). Moreover, we observe that

$$\langle SDD_{\alpha\leq 0.5}(G)\rangle \approx \langle SDD_0(G)\rangle = n(n-1)p\,.$$

However, once $\alpha > 0.5$, the curves $\langle SDD_\alpha(G)\rangle$ versus p deviate from Eq (3.1), at intermediate values of p, in the form of a bump which is enhanced the larger the value of α is. Also, in Figure 2(a) we can clearly see that Eq (3.2) is satisfied when $np \gg 1$, as expected.

Now, in Figure 2(b) we present $\langle SDD_\alpha(G)\rangle$ as a function of the probability p of ER graphs of three different sizes. It is clear from this figure that the blocks of curves, characterized by the different graph sizes (and shown in different colors), display similar curves but displaced on both axes. Moreover, the fact that these blocks of curves, plotted in semi-log scale, are shifted the same amount on both $x-$ and $y-$axis when doubling n make us anticipate the scaling of $\langle SDD_\alpha(G)\rangle$. We stress that other average variable degree-based indices on ER random graphs (normalized to the graph size) have been shown to scale with the average degree [22]. Indeed, this statement is encoded in Eq (3.4), that we derived for $np \gg 1$ but should serve as the global scaling equation for $\langle SDD_\alpha(G)\rangle$.

Therefore, in Figure 2(c) we show $\langle SDD_\alpha(G)\rangle/n$ as a function of the average degree $\langle d \rangle$ where the same curves of Figure 2(b) have been used. There we verify the global scaling of $\langle SDD_\alpha(G)\rangle$, as anticipated in Eq (3.4), by noticing that the blocks of curves (painted in different colors) for different graph sizes fall on top of each other.

Also, from Figure 2(a)–(c) we observe that the inequality of Theorem 1 is extended to the average variable symmetric division deg index on random graphs:

$$\langle SDD_\alpha(G)\rangle \leq \left\langle SDD_\beta(G)\right\rangle\,, \qquad 0 < \alpha < \beta\,; \tag{3.5}$$

see e.g., the blue arrow in Figure 2(a) which indicates increasing α. Here, the equality is attained if and only if $p = 1$. However, we have observed that $\langle SDD_\alpha(G)\rangle \approx \left\langle SDD_\beta(G)\right\rangle$ already for $\langle d \rangle \geq 10$.

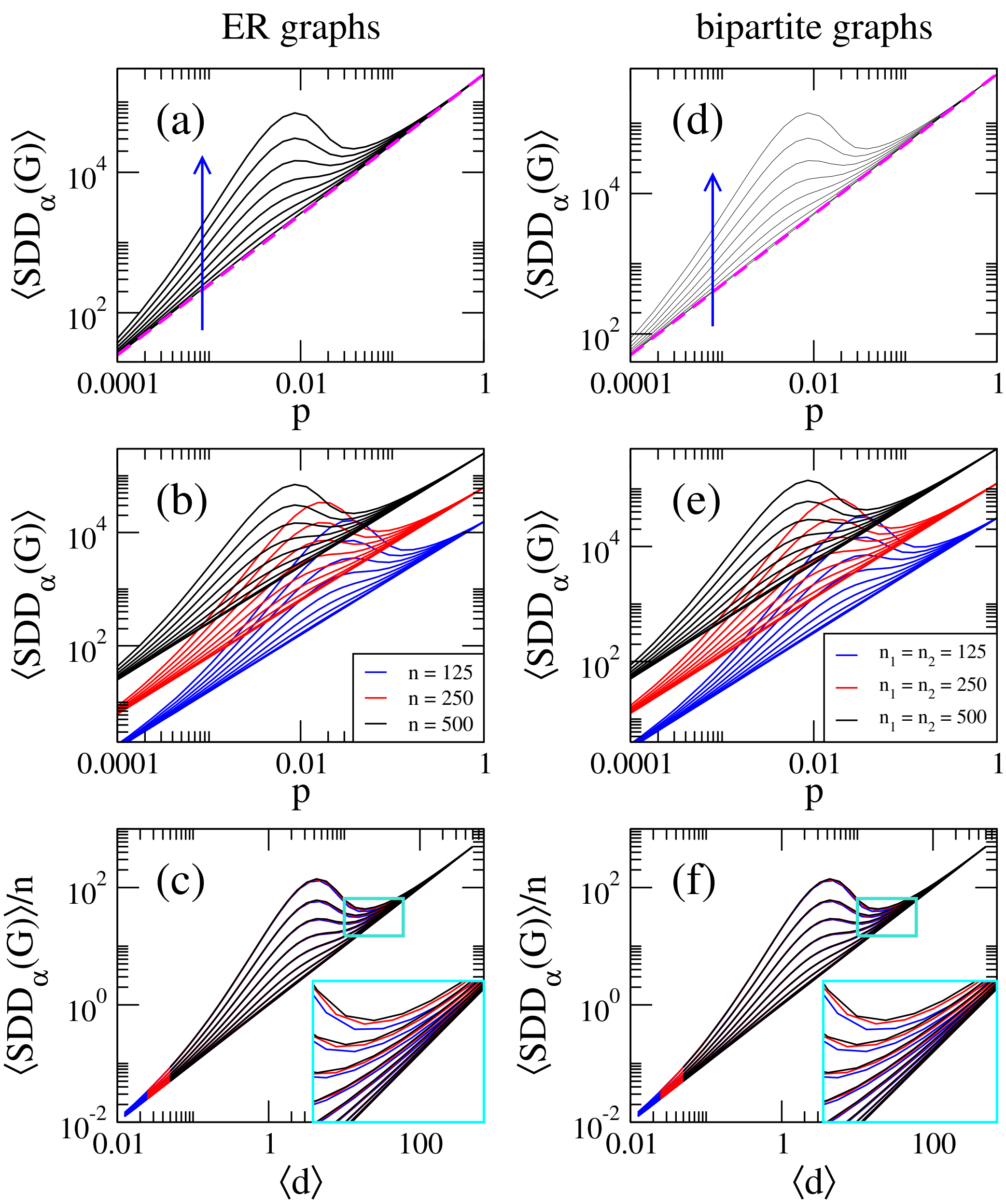

Figure 2. (a) Average variable symmetric division deg index $\langle SDD_\alpha(G)\rangle$ as a function of the probability p of Erdös-Rényi graphs of size $n = 500$. Here we show curves for $\alpha \in [0, 4]$ in steps of 0.5 (the arrow indicates increasing α). The dashed-magenta curve corresponds to the case $\alpha = 0$. (b) $\langle SDD_\alpha(G)\rangle$ as a function of the probability p of ER graphs of three different sizes: $n = 125$, 250 and 500. (c) $\langle SDD_\alpha(G)\rangle /n$ as a function of the average degree $\langle d\rangle$; same curves as in panel (b). The inset in (c) is the enlargement of the cyan rectangle. (d)–(f) Equivalent figures to (a)–(c), respectively, but for bipartite random graphs composed by sets of equal sizes: in (d) $n_1 = n_2 = 500$ while in (e),(f) $n_1 = n_2 = \{125, 250, 500\}$.

3.2. Average properties of the SDD_α index on bipartite random graphs

In Figure 2(d),(e) we present curves of the $\langle SDD_\alpha(G)\rangle$ as a function of the probability p of BR graphs. For simplicity we show results for BR graphs composed by sets of equal sizes $n_1 = n_2$. In Figure 2(d) we consider the case of $n_1 = n_2 = 500$ while in (e) we report $n_1 = n_2 = \{125, 250, 500\}$. In both figures we show curves for $\alpha \in [0, 4]$ in steps of 0.5.

Since edges in a bipartite graph join vertices of different sets, and we are labeling here the sets as sets 1 and 2, we replace d_u by d_1 and d_v by d_2 in the expression for the $SDD_\alpha(G)$ index below. Thus,

(i) For $\alpha = 0$, $\langle SDD_0(G)\rangle$ gives twice the average number of edges of the BG graph. That is,

$$\begin{aligned}\langle SDD_0(G)\rangle &= \left\langle \sum_{E(G)} \left(\frac{d_1^0}{d_2^0} + \frac{d_2^0}{d_1^0} \right) \right\rangle = \left\langle \sum_{E(G)} (1+1) \right\rangle \\ &= \langle 2|E(G)|\rangle = 2n_1 n_2 p\,. \end{aligned} \tag{3.6}$$

(ii) When both $n_1 p \gg 1$ and $n_2 p \gg 1$, we can approximate $d_1 \approx \langle d_1\rangle$ and $d_2 \approx \langle d_2\rangle$, then

$$\langle SDD_\alpha(G)\rangle \approx \left\langle \sum_{E(G)} \left(\frac{\langle d_1\rangle^\alpha}{\langle d_2\rangle^\alpha} + \frac{\langle d_2\rangle^\alpha}{\langle d_1\rangle^\alpha} \right) \right\rangle = \left\langle |E(G)| \left(\frac{\langle d_1\rangle^\alpha}{\langle d_2\rangle^\alpha} + \frac{\langle d_2\rangle^\alpha}{\langle d_1\rangle^\alpha} \right) \right\rangle. \tag{3.7}$$

(iii) In the case we consider in Figure 2(d)–(f), where $n_1 = n_2 = n/2$, so that $\langle d_1\rangle = \langle d_2\rangle = \langle d\rangle$, Equation (3.7) reduces to

$$\langle SDD_\alpha(G)\rangle \approx \langle 2|E(G)|\rangle = 2n_1 n_2 p = \frac{n^2}{2} p\,. \tag{3.8}$$

(iv) By recognizing that $\langle d\rangle = np/2$ we can rewrite Eq (3.8) as

$$\frac{\langle SDD_\alpha(G)\rangle}{n} \approx \langle d\rangle\ . \tag{3.9}$$

We stress that Eq (3.9) is expected to be valid for $np \gg 1$. We also note that Eq (3.9) has exactly the same form as Eq (3.4).

From Figure 2(d),(e) we note that

$$\langle SDD_{\alpha\le 0.5}(G)\rangle \approx \langle SDD_0(G)\rangle = 2n_1 n_2 p\,,$$

see the dashed-magenta curve in Figure 2(d). But once $\alpha > 0.5$, the curves $\langle SDD_\alpha(G)\rangle$ versus p deviate from Eq (3.6), at intermediate values of p, in the form of bumps which are enhanced the larger the value of α is. These bumps make clear the validity of inequality (3.5) on BR graphs; see e.g., the blue arrow in Figure 2(d) which indicates increasing α.

Finally, following the scaling analysis made in the previous subsection for ER graphs, in Figure 2(f) we plot the $\langle SDD_\alpha(G)\rangle/n$ as a function of the average degree $\langle d\rangle$ where the same data sets of Figure 2(e) have been used. Thus we verify that $\langle SDD_\alpha(G)\rangle$/n scales with $\langle d\rangle$, as anticipated in Eq (3.9); that is, the blocks of curves (painted in different colors) for different graph sizes coincide.

4. Conclusions

In this paper we have performed analytical and computational studies of the variable symmetric division deg index $SDD_\alpha(G)$. First, we provided a monotonicity property and obtained new inequalities connecting $SDD_\alpha(G)$ with other well–known topological indices such as the variable inverse sum deg index, as well as the the modified Narumi-Katayama index. Then, we apply the index $SDD_\alpha(G)$ on two ensembles of random graphs: Erdős-Rényi graphs and bipartite random graphs. Thus, we computationally showed, for both random graph models, that the ratio $\langle SDD_\alpha(G)\rangle /n$ is a function of the average degree $\langle d\rangle$ only (n being the order of the graph). We note that this last result, also observed for other variable topological indices [22], is valid for random bipartite graphs only when they are formed by sets of the same size.

Since many important topological indices can be written as

$$X(G) = \sum_{uv\in E(G)} F(d_u, d_v),$$

an open problem is to extend the results of this paper to other indices of this kind.

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Conflict of interest

The authors declare there is no conflict of interest.

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