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Research article

On symmetric division deg index of trees with given parameters

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Abstract: Recently, the symmetric division deg (SDD) index is proven to be a potentially useful molecular descriptor in QSAR and QSPR (quantitative structure-activity and structure-property relationships) studies. And its predictive capability is better than that of some popular topological indices, such as the famous geometric-arithmetic index and the second Zagreb index. In this work, the maximum SDD indices of trees with given matching number or domination number or independence number or number of pendant vertices or segments or diameter or radius are presented. Furthermore, the corresponding extremal trees are identified.

Keywords: symmetric division deg index; tree; matching number; domination number; segment; diameter
Mathematics Subject Classification: 05C07, 05C35, 92E10

1. Introduction

Topological molecular descriptors are mathematical invariants reflecting some biological and physico-chemical properties of organic compounds on the chemical graph, and they play a substantial role in materials science, chemistry and pharmacology, etc. (see [1–3]). Symmetric division deg (SDD for short) index is one of the 148 discrete Adriatic indices that showed good predictive properties on the testing sets provided by International Academy of Mathematical Chemistry (IAMC) [4]. This graph descriptor has a good correlation with the total surface area of polychlorobiphenyls [4] and its extremal graphs which have a particularly elegant and simple structure are obtained with the help of MathChem [5]. SDD index is defined as

$$\begin{aligned} SDD(G) &= \sum_{uv\in E(G)} \left(\frac{\min\{d_G(u), d_G(v)\}}{\max\{d_G(u), d_G(v)\}} + \frac{\max\{d_G(u), d_G(v)\}}{\min\{d_G(u), d_G(v)\}}\right) \\ &= \sum_{uv\in E(G)} \left(\frac{d_G(u)}{d_G(v)} + \frac{d_G(v)}{d_G(u)}\right), \end{aligned}$$

where $d_G(u)$ denotes the degree of vertex u in G. Recently, Furtula et al. [6] found that SDD index is an applicable and viable topological index, whose predictive capability is better than that of some popular topological indices. Gupta et al. [7] determined some upper and lower bounds of SDD index on some classes of graphs and characterized the corresponding extremal graphs. For other recent mathematical investigations, the readers can refer [8–13].

We only deal with the simple connected graphs in this work. Let $G = (V(G), E(G))$ be the graph having vertex set $V(G)$ and edge set $E(G)$. Let us denote the maxmium degree of G by $\Delta(G)$. We use $d_G(x, y)$ to denote the distance between two vertices x and y in G. Denoted by $G - uv$ the graph arising from G by deleting the edge $uv \in E(G)$. The subgraph of G obtained by deleting the vertex x ($x \in V(G)$) and its incident edges is denoted by $G - x$. Let P_n and S_n be the n-vertex path and the n-vertex star, respectively.

A matching in G is a subset $M \subseteq E(G)$ if no two edges in M are adjacent. An independent set is a subset of vertices in which no two elements are adjacent. The matching number and the independence number of a graph G is the maximum cardinality of a matching and an independent set in G, respectively. A dominating set of a graph is a vertex set $V' \subseteq V(G)$ if each vertex of $V(G) \setminus V'$ is adjacent to at least one vertex of V'. The domination number of a graph G, denoted by $\kappa(G)$, is the minimum cardinality among all dominating sets. The eccentricity $\varepsilon_G(x)$ of a vertex $x \in V(G)$ is defined as $\varepsilon_G(x) = \max\{d_G(x, y)|y \in V(G)\}$. The diameter and radius of a graph G is the maximum eccentricity and the minimum eccentricity over all vertices in G, respectively. A segment of a tree T (see [14]) is a path-subtree whose terminal vertices are pendent or branching vertices (the vertex with degree 3 or greater) of T. We can see [15] for other terminologies and notations.

2. SDD index of trees with given matching number

Denoted by $\mathscr{T}_{n,m}$ the set of trees of order n with matching number m. Thus $\mathscr{T}_{2m,m}$ are trees with a perfect matching. Let us denote the set of all pendant vertices in T by $PV(T)$.

Let $\boldsymbol{T}^*_{n,m}$ be the tree of order n obtained from S_{n-m+1} by attaching one pendant edge to each of certain $m - 1$ pendant vertices of S_{n-m+1}.

Let

$$S(x, y) = \frac{y}{x} + \frac{x}{y}, \text{ where } x, y \geq 1,$$

and

$$f(n, x) = (n - x)\left(n - \frac{3x}{2} + \frac{1}{2}\right) + \frac{5}{2}(x - 1) + \frac{n - 1}{n - x}, \text{ where } n \geq 2,\ x \geq 1 \text{ and } x \leq \frac{n}{2}.$$

One can easily get the following Lemmas 2.1−2.4.

Lemma 2.1. *Let $f_t(x) = S(x, t + 1) - S(x, t) = \frac{x}{t+1} - \frac{x}{t} + \frac{1}{x}$, where $x, t \geq 1$. Then $f_t(x)$ is decreasing for x.*

Lemma 2.2. *Let $h(t) = t + \frac{1}{t} - \frac{1}{t+1}$, where $t \geq 1$. Then $h(t)$ is increasing for t.*

Lemma 2.3. *Let T be a tree. If $d_T(x, z)$ is maximum, where $x, z \in V(T)$, then z is a pendant vertex.*

Lemma 2.4. *Let $T \in \mathscr{T}_{2m,m}$ and $y \in V(T)$. Then $| N_T(y) \cap PV(T) | \leq 1$.*

Lemma 2.5. *[16] Let $T \in \mathscr{T}_{2m,m}$. If $x, z \in V(T)$ and $d_T(x,z)$ is maximum, then z is adjacent to a vertex of degree two.*

Theorem 2.6. *Let $T \in \mathscr{T}_{2m,m}$, where $m \geq 1$. Then*

$$SDD(T) \leq f(2m,m) = \frac{m^2}{2} + 3m - \frac{1}{m} - \frac{1}{2}$$

with equality only when $T \cong \boldsymbol{T}^*_{2m,m}$.

Proof. By induction on m. If $m = 1$, $T \cong \boldsymbol{T}^*_{2,1}$ and $SDD(T) = 2 = f(2,1)$.

Suppose the theorem holds for all trees on fewer than $2m \geq 4$ vertices with a perfect matching. Let x be a vertex satisfying $d_T(x,z) = \max\{d_T(x,y), y \in V(T)\}$. Since $T \in \mathscr{T}_{2m,m}$ and $|V(T)| = 2m \geq 4$, then $d_T(x,z) \geq 3$ (notice that $d_T(x,z) = 3$ only if $T \cong P_4 \cong \boldsymbol{T}^*_{4,2}$ holds). By Lemma 2.3, it follows that z is a pendant vertex. Let $uz \in E(T)$. By lemma 2.5, $d_T(u) = 2$. Let $N_T(u) = \{v, z\}$ (v belongs to the vertices of the path from x to u in T) and $N_T(v) = \{v_1, v_2, \cdots, v_t, w\}$, where w belongs to the vertices of the path from x to v in T and $v_1 = u$ (notice that if $w = x$, then $T \cong P_4 \cong \boldsymbol{T}^*_{4,2}$). We discuss in two cases.

Case 1. $vw \notin M$.

In this case, there exists $w' \in N_T(w)$ and $v_i \in N_T(v)$ such that $ww' \in M$ and $vv_i \in M$, where $i \neq 1$. Assume without loss of generality that $vv_t \in M$. Thus it can be seen that v_t is a pendant vertex. Otherwise, there exists vertex $v'_t \in N_T(v_t) \setminus \{v\}$. By Lemma 2.4, v'_t is a pendant vertex. Since $T \in \mathscr{T}_{2m}$, we have $v_t v'_t \in M$, which contradicts $vv_t \in M$. By Lemma 2.5, we have $d_T(v_i) = 2$, $1 \leq i \leq t-1$. Let $N_T(v_i) \setminus \{v\} = \{z_i\}$, $1 \leq i \leq t-1$, where $z_1 = z$. Notice that $v_i z_i \in M$, $1 \leq i \leq t-1$. Set $T' = T - v_1 - z_1$. Thus $T' \in \mathscr{T}_{2(m-1),m-1}$. By the definition of SDD index, induction hypothesis and Lemmas 2.1, 2.2, we have

$$\begin{aligned}
SDD(T) =& SDD(T') + [S(d_T(w), d_T(v)) - S(d_T(w), d_T(v) - 1)] \\
&+ S(d_T(v_1), d_T(v)) + S(d_T(v_1), d_T(z_1)) \\
&+ \sum_{i=2}^{t-1} [S(d_T(v_i), d_T(v)) - S(d_T(v_i), d_T(v) - 1)] \\
&+ S(d_T(v_t), d_T(v)) - S(d_T(v_t), d_T(v) - 1) \\
\leq& SDD(T') + [S(2, d_T(v)) - S(2, d_T(v) - 1)] + S(2, d_T(v)) + S(2,1) \\
&+ \sum_{i=2}^{t-1} [S(2, d_T(v)) - S(2, d_T(v) - 1)] + S(1, d_T(v)) - S(1, d_T(v) - 1) \\
\leq& f(2(m-1), m-1) + (t-1)\left(\frac{1}{2} + \frac{2}{t+1} - \frac{2}{t}\right) + \frac{2}{t+1} + \frac{t}{2} + \frac{1}{2} \\
&+ \frac{5}{2} + 1 + \frac{1}{t+1} - \frac{1}{t} \\
=& f(2(m-1), m-1) + t + \frac{1}{t} - \frac{1}{t+1} + \frac{7}{2} \\
\leq& f(2(m-1), m-1) + m - 1 + \frac{1}{m-1} - \frac{1}{m} + \frac{7}{2} \\
=& f(2m, m)
\end{aligned}$$

since $t \le m-1$. With the equalities hold only if $SDD(T') = f(2(m-1), m-1)$, $t = m-1$, $d_T(w) = 2$ and $V(T) = \{w, w', v, v_t\} \cup \{v_1, v_2, \cdots, v_{t-1}\} \cup \{z_1, z_2, \cdots, z_{t-1}\}$. It implies that $T' \cong \boldsymbol{T}^*_{2(m-1),m-1}$, and $T \cong \boldsymbol{T}^*_{2m,m}$.

Case 2. $vw \in M$.

Note that $(N_T(v)\setminus\{w\}) \cap PV(T) = \emptyset$. Otherwise, for $y' \in (N_T(v)\setminus\{w\}) \cap PV(T)$, y' is not M-saturated, which contradicts $T \in \mathscr{T}_{2m,m}$. Thus we have $d_T(v_i) \ge 2$, $1 \le i \le t$. In view of Lemma 2.3, we can get that $(N_T(v_i) \setminus \{v\}) \subset PV(T)$, $1 \le i \le t$. And by Lemma 2.5, we have $d_T(v_i) = 2$, $1 \le i \le t$. Let $N_T(v_i) \setminus \{v\} = \{z_i\}$, $1 \le i \le t$, where $z_1 = z$. Notice that $v_i z_i \in M$, $1 \le i \le t$. Set $T' = T - v_1 - z_1$. Thus $T' \in \mathscr{T}_{2(m-1),m-1}$. By induction hypothesis and Lemmas 2.1, 2.2, we have

$$\begin{aligned}
SDD(T) =& SDD(T') + [S(d_T(w), d_T(v)) - S(d_T(w), d_T(v) - 1)] \\
&+ \sum_{i=2}^{t} [S(d_T(v_i), d_T(v)) - S(d_T(v_i), d_T(v) - 1)] \\
&+ S(d_T(v_1), d_T(v)) + S(d_T(v_1), d_T(z_1)) \\
\le& SDD(T') + [S(1, d_T(v)) - S(1, d_T(v) - 1)] \\
&+ \sum_{i=2}^{t} [S(2, d_T(v)) - S(2, d_T(v) - 1)] + S(2, d_T(v)) + S(2, 1) \\
\le& f(2(m-1), m-1) + \left(\frac{1}{t+1} - \frac{1}{t} + 1\right) + (t-1)\left(\frac{1}{2} + \frac{2}{t+1} - \frac{2}{t}\right) \\
&+ \frac{2}{t+1} + \frac{t+1}{2} + \frac{5}{2} \\
=& f(2(m-1), m-1) + t + \frac{1}{t} - \frac{1}{t+1} + \frac{7}{2} \\
\le& f(2(m-1), m-1) + m + \frac{1}{m-1} - \frac{1}{m} + \frac{5}{2} \\
=& f(2m, m)
\end{aligned}$$

since $t \le m-1$. With equalities hold only if $SDD(T') = f(2(m-1), m-1)$, $d_T(w) = 1$, $t = m-1$ and $V(T) = \{w, v\} \cup \{v_1, v_2, \cdots, v_t\} \cup \{z_1, z_2, \cdots, z_t\}$. It implies that $t = 1$, $w = x$ and $T' \cong \boldsymbol{T}^*_{2,1}$. Therefore we have $T \cong \boldsymbol{T}^*_{4,2}$. □

Lemma 2.7. *Let* $l(s,t) = \frac{3}{2}s + \frac{t-1}{s-1} - \frac{t}{s} = \frac{3}{2}s + \frac{t-s}{s(s-1)}$, *where* $s, t \ge 2$ *and* $s > t$. *Then* $l(s,t)$ *is increasing for* s *and* t, *respectively.*

Proof. It is evident that $l(s,t)$ is increasing for t. Furthermore, since

$$\begin{aligned}
\frac{\partial l}{\partial s} &= \frac{3}{2} - \frac{t-1}{(s-1)^2} + \frac{t}{s^2} = \frac{3}{2} + \frac{s^2 - (2s-1)t}{s^2(s-1)^2} \\
&> \frac{3}{2} + \frac{s^2 - (2s-1)s}{(s-1)^2 s^2} = \frac{3}{2} - \frac{1}{(s-1)s} \ge \frac{3}{2} - \frac{1}{2} > 0,
\end{aligned}$$

then $l(s,t)$ is increasing for s. □

Theorem 2.8. *Let $T \in \mathscr{T}_{n,m}$. Then*

$$SDD(T) \leq f(n,m).$$

The equality holds only when $T \cong \boldsymbol{T}^*_{n,m}$.

Proof. By induction on n. If $n = 2m$, by Theorem 2.6, the result holds.

Suppose the result holds for all T on fewer than n ($n > 2m$) vertices. Let M be an m-matching. Denoted by $P_{d+1} = x_1x_2\cdots x_{d+1}$ a path of length d, where d is the diameter of T. If $d \leq 2$, then $T \cong S_n \cong \boldsymbol{T}^*_{n,1}$ and $SDD(T) = f(n,1)$. In what follows, we suppose $d \geq 3$. By Lemma 2.3, we can see that x_1 is a pendant vertex. Denote $N_T(x_2) = \{x_3, u_1, u_2, \cdots, u_{r-1}\}$ and $N_T(x_3) = \{x_2, x_4, v_1, v_2, \cdots, v_{s-2}\}$, where $r, s \geq 2$ and $u_1 = x_1$. It is evident that $d_T(u_i) = 1$ $(1 \leq i \leq r-1)$. We discuss in two cases.

Case 1. $x_2x_3 \in M$.

Now $u_1 = x_1$ is not M-saturated. Set $T_1 = T - u_1$. Then $T_1 \in \mathscr{T}_{n-1,m}$. Since there exist at least $m-1$ edges for each matching in $T - \{x_2, x_3, u_1, u_2, \cdots, u_{r-1}\}$, then $n-(r+1) \geq 2(m-1)$, that is $r \leq n-2m+1$. By induction hypothesis and Lemmas 2.1, 2.2, it follows that

$$\begin{aligned}
SDD(T) =& SDD(T_1) + S(1,r) + S(s,r) - S(s,r-1) + (r-2)(S(1,r) - S(1,r-1))\\
\leq& SDD(T_1) + S(1,r) + S(2,r) - S(2,r-1) + (r-2)(S(1,r) - S(1,r-1))\\
\leq& f(n-1,m) + 2r - \frac{3}{2} - \frac{1}{r-1} + \frac{1}{r}\\
\leq& f(n-1,m) + 2(n-2m+1) - \frac{3}{2} - \frac{1}{n-2m} + \frac{1}{n-2m+1}\\
=& f(n,m) - 2n + \frac{5}{2}m + \frac{1}{2} - \frac{n-1}{n-m} + \frac{n-2}{n-m-1}\\
&+ 2(n-2m+1) - \frac{3}{2} - \frac{1}{n-2m} + \frac{1}{n-2m+1}\\
=& f(n,m) - \frac{3}{2}m - \frac{n-1}{n-m} + \frac{n-2}{n-m-1} - \frac{1}{n-2m} + \frac{1}{n-2m+1} + 1\\
<& f(n,m) - \frac{3}{2}m + \frac{m-1}{(n-m)(n-m-1)} + 1\\
<& f(n,m) - \frac{3}{2}m + \frac{3}{2}\\
<& f(n,m).
\end{aligned}$$

Case 2. $x_2x_3 \notin M$.

Since M is an m-matching in T, now there is $u_i \in N_T(x_2)$ with $x_2u_i \in M$. Without loss of generality, assume that $x_2u_1 \in M$.

Case 2.1. $r = 2$.

Set $T_2 = T - u_1 - x_2$. Then $T_2 \in \mathscr{T}_{n-2,m-1}$.

Case 2.1.1. $s = 2$.

By induction hypothesis and Lemma 2.1, it follows that

$$\begin{aligned}
SDD(T) =& SDD(T_2) + S(d(x_4),2) - S(d(x_4),1) + S(2,2) + S(2,1)\\
\leq& f(n-2,m-1) + S(2,2) - S(2,1) + 2 + \frac{5}{2}
\end{aligned}$$

$$
\begin{aligned}
&= f(n-2,m-1)+4\\
&= f(n,m)-\frac{3}{2}n+2m-\frac{n-1}{n-m}+\frac{n-3}{n-m-1}+\frac{3}{2}\\
&= f(n,m)-\frac{3}{2}n+2m-\frac{n-2m+1}{(n-m-1)(n-m)}+\frac{3}{2}\\
&\le f(n,m)-\frac{3}{2}n+2m+\frac{3}{2}\\
&\le f(n,m)-\frac{3}{2}(2m+1)+2m+\frac{3}{2}\\
&\le f(n,m)-m\\
&< f(n,m).
\end{aligned}
$$

Case 2.1.2. $s \ge 3$.

Without loss of generality, we suppose that $d(v_1) = d(v_2) = \cdots = d(v_t) = 1$ and $d(v_{t+1})$, $d(v_{t+2}), \cdots, d(v_{s-2}) \ge 2$. If $d = 3$, then $d(x_4) = 1$, $d(v_1) = d(v_2) = \cdots = d(v_{s-2}) = 1$ and this implies $T \cong \boldsymbol{T}^*_{n,2}$. So we assume that $d \ge 4$. Since there exist at least $m-3$ M-saturated vertices in $V(T)\backslash\{x_1, x_2, \cdots, x_5, v_1, v_2, \cdots, v_{s-2}\}$, then $|V(T)| = n \ge |\{x_1, x_2, \cdots, x_5, v_1, v_2, \cdots, v_{s-2}\}|+m-3 = s+m$, that is $s \le n-m$.

Case 2.1.2.1. $t \le 1$.

By induction hypothesis and Lemmas 2.1, 2.2, it follows that

$$
\begin{aligned}
SDD(T) =& SDD(T_2)+S(d(x_4),s)-S(d(x_4),s-1)+S(d(v_1),s)-S(d(v_1),s-1)\\
&+\sum_{i=2}^{s-2}(S(d(v_i),s)-S(d(v_i),s-1))+S(2,s)+S(2,1)\\
\le& f(n-2,m-1)+(s-2)(S(2,s)-S(2,s-1))\\
&+S(1,s)-S(1,s-1)+S(2,s)+S(2,1)\\
=& f(n-2,m-1)+s+\frac{5}{2}-\frac{1}{s}+\frac{1}{s-1}\\
\le& f(n,m)-\frac{3}{2}n+2m-\frac{5}{2}-\frac{n-1}{n-m}+\frac{n-3}{n-m-1}\\
&+n-m+\frac{5}{2}-\frac{1}{n-m}+\frac{1}{n-m-1}\\
=& f(n,m)-\frac{n}{2}+m-\frac{n-2m}{(n-m)(n-m-1)}\\
<& f(n,m)-\frac{n}{2}+m\\
<& f(n,m).
\end{aligned}
$$

Case 2.1.2.2. $t \ge 2$.

Since there are at least $t-1$ pendant vertices which are not M-saturated, then $n-(t-1) \ge 2m$, that is $t \le n-2m+1$. Set $T_3 = T - v_1$. Then $T_3 \in \mathscr{T}_{n-1,m}$. By induction hypothesis and Lemmas 2.1, 2.7, it follows that

$$
SDD(T) = SDD(T_3)+S(d(x_4),s)-S(d(x_4),s-1)+S(2,s)-S(2,s-1)+S(1,s)
$$

$$
\begin{aligned}
&+\sum_{i=2}^{t}(S(1,s)-S(1,s-1))+\sum_{i=t+1}^{s-2}(S(d(v_i),s)-S(d(v_i),s-1))\\
\leq& f(n-1,m)+(s-t)(S(2,s)-S(2,s-1))+S(1,s)\\
&+(t-1)(S(1,s)-S(1,s-1))\\
=& f(n-1,m)+\frac{t}{2}+\frac{3}{2}(s-2)+2-\frac{2s-t-1}{s-1}+\frac{2s-t}{s}\\
=& f(n-1,m)+\frac{t}{2}+\frac{3}{2}s-\frac{t}{s}+\frac{t-1}{s-1}-1\\
\leq& f(n-1,m)+\frac{t}{2}+\frac{3}{2}(n-m)-\frac{t}{n-m}+\frac{t-1}{n-m-1}-1\\
\leq& f(n-1,m)+\frac{n-2m+1}{2}+\frac{3}{2}(n-m)-\frac{n-2m+1}{n-m}+\frac{n-2m}{n-m-1}-1\\
=& f(n,m).
\end{aligned}
$$

The equalities hold only if $d(x_4)=2$, $t=n-2m+1$, $s=n-m$ and $T_3\cong \boldsymbol{T}^*_{n-1,m}$. This implies $T\cong \boldsymbol{T}^*_{n,m}$.

Case 2.2. $r\geq 3$.

In this case, $u_2,\cdots,u_{r-1}$ is not M-saturated and $n-(r-2)\geq 2m$, that is $r\leq n-2m+2$. Since $d\geq 3$, then $x_3x_4\in E(T)$. Set $T_4=T-u_2$. Then $T_4\in \mathscr{T}_{n-1,m}$. If $m=2$, then $T\cong \boldsymbol{T}^*_{n,2}$. If $m\geq 3$, By induction hypothesis and Lemmas 2.1, 2.2, it follows that

$$
\begin{aligned}
SDD(T)=& SDD(T_4)+S(d(x_3),r)-S(d(x_3),r-1)+S(1,r)-S(1,r-1)+S(1,r)\\
&+\sum_{i=3}^{r-1}(S(1,r)-S(1,r-1))\\
\leq& f(n-1,m)+S(2,r)-S(2,r-1)+(r-2)(S(1,r)-S(1,r-1))+S(1,r)\\
=& f(n-1,m)+2r+\frac{1}{r}-\frac{1}{r-1}-\frac{3}{2}\\
\leq& f(n-1,m)+2(n-2m+2)+\frac{1}{n-2m+2}-\frac{1}{n-2m+1}-\frac{3}{2}\\
<& f(n-1,m)+2(n-2m+2)-\frac{3}{2}\\
=& f(n,m)-\frac{3}{2}m+3+(m-1)\left(\frac{1}{n-m-1}-\frac{1}{n-m}\right)\\
<& f(n,m)-\frac{3}{2}m+3+\frac{1}{3}\\
<& f(n,m)
\end{aligned}
$$

since $\frac{1}{n-m-1}-\frac{1}{n-m}<\frac{1}{m-1}-\frac{1}{m}$ for $n-m>m$ $(n>2m)$.

The proof is completed. □

Suppose G ia a bipartite graph on n vertices with matching number m and independence number β. That, as we all know, $m+\beta=n$ for any bipartite graph G, see [15]. Since a tree is a bipartite graph, by Theorem 2.8, the Theorem 2.9 is immediate.

Theorem 2.9. *Suppose T is a tree on n vertices with independence number β. Then*

$$SDD(T) \leq f(n, n-\beta).$$

With equality if and only if $T \cong \boldsymbol{T}^*_{n,n-\beta}$.

3. SDD index of trees with given domination number

It is evident that $\kappa(T) = 1$ for a tree T on n vertices if and only if $T \cong S_n$. It is well known that for a graph G on n vertices, $\kappa(G) \leq \frac{n}{2}$ [17]. Fink et al [18] determined the n-vertex graphs G with $\kappa(G) = \frac{n}{2}$. Let $\mathbf{T}_{n,\kappa}$ be the n-vertex trees with domination number κ. Note that for $T \in \mathbf{T}_{n,\kappa}$ with $\Delta(T) = n - \kappa$, then $T \cong \boldsymbol{T}^*_{n,\kappa}$.

Theorem 3.1. *Let $T \in \mathbf{T}_{n,\kappa}$, where $n \geq 3$ and $\kappa \leq \frac{n}{2}$. Then*

$$SDD(T) \leq f(n, \kappa).$$

The equality holds only when $T \cong \boldsymbol{T}^*_{n,\kappa}$.

Proof. If $n = 3$, $T \cong P_3 \cong \boldsymbol{T}^*_{3,1}$ and $SDD(P_3) = 5 = f(3, 1)$. If $n = 4$, $T \cong P_4 \cong \boldsymbol{T}^*_{4,2}$ or $S_4 \cong \boldsymbol{T}^*_{4,1}$, and $SDD(P_4) = 7 = f(4, 2)$, $SDD(S_4) = 10 = f(4, 1)$. Now, suppose $n \geq 5$ and the theorem holds for any T on fewer than n vertices. We use $P_{d+1} = x_1x_2 \cdots x_{d+1}$ to denote a path of length d, where d is the diameter of T. If $d = 2$, then $T \cong S_n$ and $\kappa(S_n) = 1$, the result is ture. So in what follows, we suppose that $\kappa(T) \geq 2$. Denote $N_T(x_2) = \{x_1, x_3, u_1, u_2, \cdots, u_{r-2}\}$ and $N_T(x_3) = \{x_2, x_4, v_1, v_2, \cdots, v_{s-2}\}$, where $r, s \geq 2$. Set $T_1 = T - \{x_1\}$.

Case 1. $\kappa(T_1) = \kappa(T)$.

By the definition of SDD index, induction hypothesis and Lemma 2.1, it follows that

$$\begin{aligned} SDD(T) =& SDD(T_1) + S(1, r) + S(r, s) - S(r-1, s) + (r-2)(S(1, r) - S(1, r-1)) \\ \leq& f(n-1, \kappa) + S(1, r) + S(r, 2) - S(r-1, 2) + (r-2)(S(1, r) - S(1, r-1)) \\ =& f(n, \kappa) - 2n + \frac{5}{2}\kappa + \frac{1}{2} + \frac{n-2}{n-\kappa-1} - \frac{n-1}{n-\kappa} + 2r + \frac{1}{r} - \frac{1}{r-1} - \frac{3}{2}. \end{aligned}$$

Since $\kappa \leq \frac{n-(r-2)}{2}$, that is $r \leq n - 2\kappa + 2$, by Lemma 2.2, it follows that

$$\begin{aligned} SDD(T) \leq& f(n, \kappa) - 2n + \frac{5}{2}\kappa + \frac{1}{2} + \frac{n-2}{n-\kappa-1} - \frac{n-1}{n-\kappa} + 2(n - 2\kappa + 2) \\ &+ \frac{1}{n-2\kappa+2} - \frac{1}{n-2\kappa+1} - \frac{3}{2} \\ =& f(n, \kappa) - \frac{3}{2}\kappa + 3 + \frac{n-2}{n-\kappa-1} - \frac{n-1}{n-\kappa} + \frac{1}{n-2\kappa+2} - \frac{1}{n-2\kappa+1}. \end{aligned}$$

If $\kappa = 2$, $SDD(T) \leq f(n, \kappa)$. The equalities hold if only $s = 2$ and $n = r + 2$. This implies $T \cong \boldsymbol{T}^*_{n,2}$. If $\kappa \geq 3$, we have

$$SDD(T) < f(n, \kappa) - \frac{3}{2}\kappa + 3 + \frac{n-2}{n-\kappa-1} - \frac{n-1}{n-\kappa}$$

$$=f(n,\kappa)-\frac{3}{2}\kappa+3+\frac{\kappa-1}{(n-\kappa)(n-\kappa-1)}.$$

Since $\frac{\kappa-1}{(n-\kappa)(n-\kappa-1)}<1$, then for $\kappa\geq 3$, $SDD(T)<f(n,\kappa)-\frac{3}{2}\kappa+4<f(n,\kappa)-\frac{1}{2}<f(n,\kappa)$.

Case 2. $\kappa(T_1)=\kappa(T)-1$.

In this case, we have $r=2$, otherwise x_2 belongs to each minimum dominating set and implies $\kappa(T_1)=\kappa(T)$. For $s=n-\kappa$, then $T\cong \boldsymbol{T}^*_{n,\kappa}$, and the theorem holds. So in what follows, we assume that $s\leq n-\kappa-1$. By the case 1 above, assume that $d(v_i)\leq 2$, $i\in\{1,2,\cdots,s-2\}$. If x_4 is a pendant vertex or a support vertex with $d(x_4)=2$, then $T\cong \boldsymbol{T}^*_{n,\kappa}$. In other cases, without loss of generality, let $d(v_1)=\cdots=d(v_{s_1})=1$, $d(v_{s_1+1})=\cdots=d(v_{s_1+s_2})=2$, where $s_1+s_2=s-2$.

Case 2.1. $s_1\geq 2$.

Set $T_2=T-\{v_1\}$. Then $\kappa(T_2)=\kappa(T)$. By the definition of SDD index, induction hypothesis and Lemma 2.1, it follows that

$$\begin{aligned}SDD(T)=&SDD(T_2)+S(s,2)-S(s-1,2)+S(s,1)+S(s,d(x_4))-S(s-1,d(x_4))\\&+(s_1-1)(S(s,1)-S(s-1,1))+s_2(S(s,2)-S(s-1,2))\\\leq&SDD(T_2)+s+\frac{1}{s}+(s_1-1)\Big(1+\frac{1}{s}-\frac{1}{s-1}\Big)+(s_2+2)\Big(\frac{1}{2}+\frac{2}{s}-\frac{2}{s-1}\Big)\\\leq&f(n,\kappa)-2n+\frac{5}{2}\kappa+\frac{1}{2}-\frac{n-1}{n-\kappa}+\frac{n-2}{n-\kappa-1}+\frac{3}{2}s+\frac{s_1}{2}-1+\frac{s_1-s}{s(s-1)}\\<&f(n,\kappa)-2n+\frac{5}{2}\kappa+\frac{1}{2}-\frac{n-1}{n-\kappa}+\frac{n-2}{n-\kappa-1}+\frac{3}{2}s+\frac{s_1}{2}-1.\end{aligned}$$

Since $s\leq n-\kappa-1$, $\kappa\leq\frac{n-(s_1-1)}{2}$ and $-\frac{n-1}{n-\kappa}+\frac{n-2}{n-\kappa-1}=\frac{\kappa-1}{(n-\kappa)(n-\kappa-1)}<1$. Therefore

$$\begin{aligned}SDD(T)<&f(n,\kappa)-2n+\frac{5}{2}\kappa+\frac{1}{2}+\frac{3}{2}(n-\kappa-1)+\frac{n-2\kappa+1}{2}\\=&f(n,\kappa)-\frac{1}{2}<f(n,\kappa).\end{aligned}$$

Case 2.2. $s_1\leq 1$.

Set $T_3=T-\{x_1,x_2\}$. By the definition of SDD index, induction hypothesis and Lemma 2.1, it follows that

$$\begin{aligned}SDD(T)=&SDD(T_3)+S(s,d(x_4))-S(s-1,d(x_4))+S(s,d(v_1))-S(s-1,d(v_1))\\&+S(s,2)+S(1,2)+(s-3)(S(s,2)-S(s-1,2))\\\leq&SDD(T_3)+1+\frac{1}{s}-\frac{1}{s-1}+\Big(\frac{s}{2}+\frac{2}{s}\Big)+\frac{5}{2}+(s-2)\Big(\frac{1}{2}+\frac{2}{s}-\frac{2}{s-1}\Big)\\\leq&f(n-2,\kappa-1)+s+\frac{5}{2}+\frac{1}{s-1}-\frac{1}{s}\\\leq&f(n,\kappa)-\frac{3}{2}n+2\kappa-\frac{5}{2}-\frac{n-1}{n-\kappa}+\frac{n-3}{n-\kappa-1}+s+\frac{5}{2}+\frac{1}{s-1}-\frac{1}{s}.\end{aligned}$$

Since $s\leq n-\kappa-1$, $\frac{1}{s-1}-\frac{1}{s}=\frac{1}{s(s-1)}\leq\frac{1}{2}$ and $-\frac{n-1}{n-\kappa}+\frac{n-3}{n-\kappa-1}=\frac{2\kappa-n-1}{(n-\kappa)(n-\kappa-1)}<0$. Therefore

$$SDD(T)<f(n,\kappa)-\frac{3}{2}n+2\kappa+n-\kappa-1+\frac{1}{2}$$

$$
\begin{aligned}
&= f(n,\kappa) - \frac{n}{2} + \kappa - \frac{1}{2}\\
&\le f(n,\kappa) - \frac{1}{2} < f(n,\kappa).
\end{aligned}
$$

The proof is completed. □

4. SDD index of trees with given segments or number of pendant vertices

Let $\boldsymbol{T}^{(1)}_{n,s}$ and $\boldsymbol{T}^{(2)}_{n,p}$ be the n-vertex trees with s segments and p pendant vertices, respectively. $\boldsymbol{T}^{(1)}_{n,1}$ is a path, $\boldsymbol{T}^{(1)}_{n,2}$ is empty and $\boldsymbol{T}^{(1)}_{n,n-1}$ is a tree containing no vertex of degree 2 (see [19]). In [18], Vasilyev proved that S_n has the maximum SDD index for any tree T on n vertices, so S_n also has the maximum SDD index for $T \in \boldsymbol{T}^{(1)}_{n,n-1}$. Furthermore, $\boldsymbol{T}^{(2)}_{n,2}$ is a path, $\boldsymbol{T}^{(2)}_{n,n-1}$ is star. Thus we only consider the case of $3 \le s \le n-2$ ($3 \le p \le n-2$, respectively) when $T \in \boldsymbol{T}^{(1)}_{n,s}$ ($T \in \boldsymbol{T}^{(2)}_{n,p}$, respectively). Let

$$
g(n,x) = 2n + x^2 - \frac{5}{2}x - \frac{1}{2} + \frac{1}{x}, \text{ where } n \ge 5 \text{ and } 2 \le x \le n-2.
$$

Let $\mathcal{T}_{n,s}$ be the tree of order n obtained from P_{n-s+1} by attaching $s-1$ pendant edge to one pendant vertex of P_{n-s+1}.

Theorem 4.1. *Let $T \in \boldsymbol{T}^{(1)}_{n,s}$, where $n \ge 5$ and $3 \le s \le n-2$. Then*

$$
SDD(T) \le g(n,s)
$$

with equality only when $T \cong \mathcal{T}_{n,s}$.

Proof. By induction on n. If $n = 5$, then $s = 3$, $T \cong \mathcal{T}_{5,3}$ and $SDD(\mathcal{T}_{5,3}) = g(5,3)$, the result holds. Now, suppose $n \ge 6$ and the result holds for any T of order $n-1$. Denoted by $P_{d+1} = x_1x_2\cdots x_{d+1}$ a path of length d, where d is the diameter of T. If $d = 2$, then $T \cong S_n$. Therefore $d \ge 3$. Set $T' = T - \{x_1\}$.

Case 1. $d(x_2) = 2$.

Then $T' \in \boldsymbol{T}^{(1)}_{n-1,s}$. By induction hypothesis and Lemma 2.1, it follows that

$$
\begin{aligned}
SDD(T) &= SDD(T') + S(1,2) + S(2, d(x_3) - S(1, d(x_3))\\
&\le g(n-1,s) + S(2,2)\\
&= g(n,s).
\end{aligned}
$$

With equality only when $d(x_3) = 2$ and $T' \cong \mathcal{T}_{n-1,s}$. This implies $T \cong \mathcal{T}_{n,s}$.

Case 2. $d(x_2) \ge 3$.

Denote $N_T(x_2) \setminus \{x_1, x_3\} = \{u_1, u_2, \cdots, u_t\}$, where $t \ge 1$. Then $u_1, u_2, \cdots, u_t$ are pendant vertices and $T' \in \boldsymbol{T}^{(1)}_{n-1,s-1}$. Since $t \le s-2$, by induction hypothesis and Lemmas 2.1, 2.2, it follows that

$$
\begin{aligned}
SDD(T) =& SDD(T') + S(1,t+2) + \sum_{i=1}^{t}(S(t+2,d(u_i)) - S(t+1,d(u_i)))\\
&+ S(t+2,d(x_3)) - S(t+1,d(x_3))\\
\le& g(n-1,s-1) + S(1,t+2) + t(S(t+2,1) - S(t+1,1))
\end{aligned}
$$

$$
\begin{aligned}
&+S(t+2,2)-S(t+1,2)\\
=&g(n-1,s-1)+2t+\frac{5}{2}+\frac{1}{t+2}-\frac{1}{t+1}\\
\leq&g(n-1,s-1)+2(s-2)+\frac{5}{2}+\frac{1}{s}-\frac{1}{s-1}\\
=&g(n,s).
\end{aligned}
$$

The equalities hold if only $d(x_3)=2$ and $T'\cong\mathcal{T}_{n-1,s-1}$. This implies $T\cong\mathcal{T}_{n,s}$. □

By a similar proof of Theorem 4.1, we can get Theorem 4.2.

Theorem 4.2. *Let $T\in\boldsymbol{T}^{(2)}_{n,p}$, where $n\geq 5$ and $3\leq p\leq n-2$. Then*

$$SDD(T)\leq g(n,p)$$

with equality if and only if $T\cong\mathcal{T}_{n,p}$.

5. SDD index of trees with given diameter

Let $\boldsymbol{T}^{(3)}_{n,d}$ be the n-vertex trees with diameter d. Since $\boldsymbol{T}^{(3)}_{n,2}\cong S_n$, so we consider the case of $3\leq d\leq n-1$ when $T\in\boldsymbol{T}^{(3)}_{n,d}$.

Theorem 5.1. *Let $T\in\boldsymbol{T}^{(3)}_{n,d}$, where $3\leq d\leq n-1$. Then*

$$SDD(T)\leq g(n,n-d+1)$$

with equality only when $T\cong\mathcal{T}_{n,n-d+1}$.

Proof. By induction on n. If $n=4$, then $d=3$, $T\cong P_4\cong\mathcal{T}_{4,2}$ and $SDD(P_4)=g(4,2)$, the result holds. Now, suppose $n\geq 5$ and the theorem holds for any T on $n-1$ vertices. We use $P_{d+1}=x_1x_2\cdots x_{d+1}$ to denote a path of length d in T. Set $T'=T-\{x_1\}$.

Case 1. $d(x_2)=2$.

If the diameter of T' is d, since $1\leq n-d\leq n-3$, by induction hypothesis and Lemma 2.1, it follows that

$$
\begin{aligned}
SDD(T)=&SDD(T')+S(1,2)+S(2,d(x_3)-S(1,d(x_3))\\
\leq&g(n-1,n-d)+S(2,2)\\
=&g(n,n-d+1)-2(n-d)+\frac{3}{2}-\frac{1}{n-d+1}+\frac{1}{n-d}\\
\leq&g(n,n-d+1)-2+\frac{3}{2}+1-\frac{1}{2}\leq g(n,n-d+1).
\end{aligned}
$$

The equalities hold if only $d(x_3)=2$, $n-d=1$ and $T'\cong\mathcal{T}_{n-1,n-d}$. But these cannot hold together, so $SDD(T)<g(n,n-d+1)$.

If the diameter of T' is $d-1$, by induction hypothesis and Lemma 2.1, it follows that

$$SDD(T)\leq g(n-1,n-d+1)+S(2,2)$$

$$=g(n, n-d+1).$$

The equality holds if only $d(x_3) = 2$ and $T' \cong \mathcal{T}_{n-1,n-d+1}$. This implies $T \cong \mathcal{T}_{n,n-d+1}$.

Case 2. $d(x_2) \geq 3$.

Denote $N_T(x_2) \setminus \{x_1, x_3\} = \{u_1, u_2, \cdots, u_t\}$, where $t \geq 1$ and $u_1, u_2, \cdots, u_t$ are pendant vertices. Then the diameter of T' is d. Since $t \leq n - (d + 1)$, by induction hypothesis and Lemmas 2.1, 2.2, we have

$$\begin{aligned}
SDD(T) =& SDD(T') + S(1, t+2) + \sum_{i=1}^{t} (S(t+2, d(u_i)) - S(t+1, d(u_i))) \\
&+ S(t+2, d(x_3)) - S(t+1, d(x_3)) \\
\leq& g(n-1, n-d) + 2t + \frac{5}{2} + \frac{1}{t+2} - \frac{1}{t+1} \\
\leq& g(n-1, n-d) + 2(n-d-1) + \frac{5}{2} - \frac{1}{n-d} + \frac{1}{n-d+1} \\
=& g(n, n-d+1).
\end{aligned}$$

The equalities hold if only $d(x_3) = 2$ and $T' \cong \mathcal{T}_{n-1,n-d}$. This implies $T \cong \mathcal{T}_{n,n-d+1}$. $\square$

The center of a tree T is the set of vertices with minimum eccentricity (see [14]). A tree T has exactly one or two adjacent center vertices. Let d and r be the diameter and radius of T, respectively. Then

$$d = \begin{cases} 2r-1, & \text{if } T \text{ is bicentral,} \\ 2r, & \text{if } T \text{ has unique center vertex.} \end{cases}$$

We can easily conclude that $SDD(\mathcal{T}_{n,n-2r+2}) > SDD(\mathcal{T}_{n,n-2r+1})$. Thus we have the following Theorem 5.2.

Theorem 5.2. *Let T be a tree of order n with radius r, where $2 \leq r \leq \frac{n-1}{2}$. Then*

$$SDD(T) \leq g(n, n-2r+2)$$

with equality if and only if $T \cong \mathcal{T}_{n,n-2r+2}$.

6. Conclusions

The mathematical properties of SDD index deserves further study since it can be applied in detecting the chemical compounds which may have desirable properties. SDD index has been studied extensively since it was proved to be an applicable and viable molecular descriptor in 2018. In this paper, by analyzing the vertex degree of the path whose length is the diameter in a tree and using the method of mathematical induction, we present the maximum SDD indices of trees with given matching number or independence number or domination number or segments or diameter or radius or number of pendant vertices, and identify the corresponding extremal trees. It can be seen that SDD index is in a manner a (local) measure of irregularity. Thus, by adding the pendant vertices as much as possible on the maximum degree vertex to increase the irregularity in a tree with given parameter, one can also explore the extremal trees with other given parameters.

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Conflict of interest

The authors declare no conflict of interest.

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