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ON INVERSE SYMMETRIC DIVISION DEG INDEX OF GRAPHS

Zahid Raza[1], Laxman Saha[2] and Kinkar Chandra Das[3,*]

Abstract. One of the 148 discrete Adria indices is the symmetric division deg (SDD) index. It was developed about 13 years ago. Motivated by the success of the symmetric division deg index, Ghorbani *et al.* recently proposed an inverse version of this index, which they called the ISDD index (Inverse symmetric division deg index). The inverse symmetric division deg index (ISDD) of a graph Γ is defined as follows:

$$\mathrm{ISDD}(\Gamma)=\sum_{v_iv_j\in E(\Gamma)}\frac{d_id_j}{d_i^2+d_j^2},$$

where d_i is the degree of the vertex v_i in Γ. In this paper, we determine the second maximal and the second minimal trees with respect to the inverse symmetric division deg index (ISDD). We prove that the star gives the minimal and the complete bipartite graph $K_{\lceil \frac{n}{2}\rceil,\lfloor \frac{n}{2}\rfloor}$ gives the maximal graphs with respect to the inverse symmetric division deg index (ISDD) among any chain graph of order n. Moreover, the Turán graph gives the maximal graph with respect to the ISDD index for any simple graph of order n with chromatic number k. Finally, we give concluding remarks about future works.

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1. Introduction

Let $\Gamma=(V,E)$ be a simple graph having n vertices and m edges, where $V(\Gamma)=\{v_1,v_2,\ldots,v_n\}$ with $|V(\Gamma)|=n$, $|E(\Gamma)|=m$. The degree of the vertex v_i, denoted by d_i, is the number of edges incident to v_i. In particular, the maximum and minimum degrees of the graph Γ are denoted by $\Delta(\Gamma)$ and $\delta(\Gamma)$, respectively. The neighbor set of the vertex v_i is denoted by $N_\Gamma(v_i)$, that is, $|N_\Gamma(v_i)|=d_i$. We write $v_iv_j\in E(\Gamma)$ if vertices v_i and v_j are adjacent in Γ. Let d_{ij} be the shortest distance between vertices v_i and v_j in Γ. Also let d be the diameter in Γ, that is, $d=\max_{1\le i<j\le n} d_{ij}$. A topological index I of a graph Γ is the function defined on the set of all graphs that satisfies the equation $I(\Gamma)=I(H)$ whenever Γ is isomorphic to H. The graph theoretic definitions can be found in the book [5].

Particularly in QSPR/QSAR studies, molecular descriptors are crucial in mathematical chemistry. Among them, the so-called topological descriptors occupy a special place. Nowadays, several topological indices exist

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[1] Department of Mathematics, College of Sciences, University of Sharjah, 27272 Sharjah, UAE.

[2] Department of Mathematics, Balurghat College, Balurghat 733101, India.

[3] Department of Mathematics, Sungkyunkwan University, Suwon 16419, Republic of Korea.

*Corresponding author: kinkardas2003@gmail.com

with applications in chemistry. They can be categorised based on the structural properties of the graphs used for their calculation. In the literature there were so many indices have been studied and their relation with physical properties of the some chemical compounds. Therefore, the oldest and the most popular distance based topological index, Wiener index [31] is based on the topological distance of the vertices of the corresponding graph; the Hosoya index [24] is calculated by counting non-incident edges in a graph; energy [11, 12, 25] and Estrada index [9, 15, 17] are based on the graphical spectrum; Randić connectivity index [29], Zagreb indices [6, 8, 23], geometric-arithmetic index [13], atom-bond connectivity index [16, 18, 20], harmonic index [19] are calculated using the degrees of vertices, etc. Very recently, some researchers studied on the degree based topological indices in terms of graph parameters [1, 27, 32].

To enhance QSPR/QSAR studies, the authors of [30] investigated a new class of topological indices, the "discrete Adriatic indices" consisting of 148 indices. The symmetric division deg (SDD) index is one of such handful indices; for a graph Γ, the SDD index is defined as

$$\mathrm{SDD}(\Gamma) = \sum_{v_iv_j \in E(\Gamma)} \frac{d_i^2 + d_j^2}{d_i d_j}.$$

A rigorous multidimensional investigation of the SDD index has been carried out by Furtula *et al.* [21] and it was found that SDD is a feasible and practical topological index. This index performed much better than that of several other popular topological indices. Since then, there are so many paper specially related with SDD has been published, see for example [3, 10].

In response to the popularity of the SDD index, Ghorbani *et al.* [22] introduced the ISDD (inverse symmetric division deg) index, which is the inverse version of the SDD index. The ISDD index of a graph Γ is defned as follows:

$$\mathrm{ISDD}(\Gamma) = \sum_{v_iv_j \in E(\Gamma)} \frac{d_i d_j}{d_i^2 + d_j^2}.$$

The maximum and minimum trees of fixed order with respect to ISSD index have been characterized completely in [22]. Albalahi and Ali [2] addressed the problem of finding the graphs having the largest and smallest ISDD index from the set of all connected unicyclic graphs having the specified order. Throughout this paper we use P_n, S_n, C_n, $K_{p,q}\,(p+q=n)$ and K_n to denote the path graph, star graph, cycle graph, complete bipartite graph and complete graph on n vertices, respectively.

This paper is scheduled as follows. In Section 2, we list some previously known results. In Section 3, we determine the second maximal and the second minimal of the ISDD index of trees. In Section 4, we prove that star gives the minimal and the complete bipartite graph $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$ gives the maximal chain graphs of order n. In Section 5, the turan graph gives the maximal graph with respect to the ISDD index for any simple graph of order n with chromatic number k. In Section 6, we give concluding remarks with future works.

2. Preliminaries

We provide a list of some previously known results that are necessary for the following three sections.

Lemma 2.1 ([28])**.** *Let $p > 0$ and b_k, $y_k > 0$ for $1 \le k \le r$. Then*

$$\sum_{k=1}^{r} \frac{y_k^{p+1}}{b_k^p} \ge \frac{\left(\sum_{k=1}^{r} y_k\right)^{p+1}}{\left(\sum_{k=1}^{r} b_k\right)^p}$$

with equality iff $\frac{y_1}{b_1} = \frac{y_2}{b_2} = \cdots = \frac{y_r}{b_r}$.

Lemma 2.2. *The weighted AM-HM inequality relates the weighted arithmetic and harmonic means. It states that for any list of weights* $a_1, a_2, \ldots, a_n \geq 0$ *such that* $a_1 + a_2 + \cdots + a_n = a$*,*

$$\frac{a_1\, y_1 + a_2\, y_2 + \cdots + a_n\, y_n}{a} \geq \frac{a}{\frac{a_1}{y_1} + \frac{a_2}{y_2} + \cdots + \frac{a_n}{y_n}}$$

with equality iff $y_1 = y_2 = \cdots = y_n$*.*

The following conclusion is obtained from the proof of Theorem 2.3 in [7].

Lemma 2.3 ([7])**.** *Let* $v_i v_j$ *be any edge in* Γ *with* $d_i \geq d_j$*. Then*

$$\frac{d_i\, d_j}{d_i^2 + d_j^2} \geq \frac{\Delta\, \delta}{\Delta^2 + \delta^2},$$

where Δ *is the maximum degree and* δ *is the minimum degree in* Γ*. Moreover, the equality holds iff* $(d_i,\, d_j) = (\Delta,\, \delta)$*.*

Lemma 2.4. *Let* $v_i v_j$ *be any edge in* Γ *with* $d_i \geq d_j$*. Then*

$$\frac{d_i\, d_j}{d_i^2 + d_j^2} \leq \frac{1}{2}$$

with equality iff $d_i = d_j$*.*

Proof. Since $(d_i - d_j)^2 \geq 0$, we obtain

$$\frac{d_i\, d_j}{d_i^2 + d_j^2} \leq \frac{1}{2}.$$

Moreover, the equality holds iff $d_i = d_j$. □

From the above result, we obtain the maximum value of $\frac{d_i\, d_j}{d_i^2 + d_j^2}$ is 1/2. So now we want to find the second maximum value of $\frac{d_i\, d_j}{d_i^2 + d_j^2}$ in the following result:

Lemma 2.5. *Let* $v_i v_j$ *be any edge in* Γ *with* $d_i > d_j$*. Then*

$$\frac{d_i\, d_j}{d_i^2 + d_j^2} \leq \frac{\Delta\, (\Delta - 1)}{\Delta^2 + (\Delta - 1)^2},$$

where Δ *is the maximum degree of graph* Γ*. Moreover, the equality holds iff* $d_i = \Delta$ *and* $d_j = \Delta - 1$*.*

Proof. Let $v_i v_j$ be any edge in Γ such that $d_i > d_j$. Since Δ is the maximum degree in Γ and $d_i > d_j$, we obtain

$$(d_i - d_j)\, \Delta \geq d_i, \quad \text{that is, } \frac{d_i}{d_j} \geq \frac{\Delta}{\Delta - 1}$$

with equality iff $d_i = \Delta$ and $d_j = \Delta - 1$. From the above, we obtain

$$\sqrt{\frac{d_i}{d_j}} \geq \sqrt{\frac{\Delta}{\Delta - 1}} \quad \text{and} \quad \sqrt{\frac{d_j}{d_i}} \leq \sqrt{\frac{\Delta - 1}{\Delta}},$$

that is,

$$\sqrt{\frac{d_i}{d_j}} - \sqrt{\frac{d_j}{d_i}} \geq \sqrt{\frac{\Delta}{\Delta - 1}} - \sqrt{\frac{\Delta - 1}{\Delta}},$$

that is,

$$\left(\sqrt{\frac{d_i}{d_j}}-\sqrt{\frac{d_j}{d_i}}\right)^2 \geq \left(\sqrt{\frac{\Delta}{\Delta-1}}-\sqrt{\frac{\Delta-1}{\Delta}}\right)^2,$$

that is,

$$\frac{d_i}{d_j}+\frac{d_j}{d_i} \geq \frac{\Delta}{\Delta-1}+\frac{\Delta-1}{\Delta},$$

that is,

$$\frac{d_i\,d_j}{d_i^2+d_j^2} \leq \frac{\Delta\,(\Delta-1)}{\Delta^2+(\Delta-1)^2}.$$

Moreover, the equality holds iff $d_i=\Delta$ and $d_j=\Delta-1$. □

3. ISDD index on trees

Recall that $\mathrm{DS}_{r,t}$ $(r+t=n-2,\ r\geq t\geq 1)$, a double star of order n, obtained from joining the center of two stars S_{r+1} and S_{t+1}. We now give a lower bound on ISDD in terms of n of any tree $T\,(\ncong S_n)$ and characterize the corresponding extremal graphs.

Theorem 3.1. *Let $T\,(\ncong S_n)$ be a tree of order n. Then*

$$\mathrm{ISDD}(T) \geq \frac{(n-2)\,(n-3)}{(n-2)^2+1}+\frac{2}{5}+\frac{2\,(n-2)}{(n-2)^2+4}$$

with equality iff $T\cong \mathrm{DS}_{n-3,1}$.

Proof. Let Δ be the maximum degree in tree T. Since $T\ncong S_n$, we have $\Delta\leq n-2$. Let d be the diameter of tree T. We have $d\geq 3$. We take into account the next two scenarios:

Case 1. $d=3$. In this case $T\cong \mathrm{DS}_{r,t}$ $(r+t=n-2,\ r\geq t\geq 1)$. Now,

$$\begin{aligned}\mathrm{ISDD}(\mathrm{DS}_{r,t}) &= \frac{(r+1)\,r}{(r+1)^2+1}+\frac{(t+1)\,t}{(t+1)^2+1}+\frac{(r+1)\,(t+1)}{(r+1)^2+(t+1)^2}\\ &= \frac{(n-t-1)\,(n-t-2)}{(n-t-1)^2+1}+\frac{(t+1)\,t}{(t+1)^2+1}+\frac{(n-t-1)\,(t+1)}{(n-t-1)^2+(t+1)^2}.\end{aligned} \tag{1}$$

Let us consider a function

$$h(y)=\frac{(n-y-1)\,(n-y-2)}{(n-y-1)^2+1}+\frac{(y+1)\,y}{(y+1)^2+1}+\frac{(n-y-1)\,(y+1)}{(n-y-1)^2+(y+1)^2},\quad 1\leq y\leq \left\lfloor\frac{n}{2}\right\rfloor-1.$$

Then we have

$$\begin{aligned}h'(y) &= -\frac{(n-y-1)\,(n-y+1)-1}{\left[(n-y-1)^2+1\right]^2}+\frac{(y+1)^2+2(y+1)-1}{\left[(y+1)^2+1\right]^2}+\frac{n^2\,(n-2y-2)}{\left[(n-y-1)^2+(y+1)^2\right]^2}\\ &\geq -\frac{a\,(a+2)-1}{(a^2+1)^2}+\frac{b^2+2b-1}{(b^2+1)^2},\end{aligned} \tag{2}$$

where $a=n-y-1$ and $b=y+1$. Since $1\leq y\leq \lfloor\frac{n}{2}\rfloor-1$, one can easily see that $a\geq\lceil\frac{n}{2}\rceil\geq\lfloor\frac{n}{2}\rfloor\geq b\geq 2$. Now we have to prove that

$$\frac{b^2+2b-1}{(b^2+1)^2}\geq\frac{a\,(a+2)-1}{(a^2+1)^2},$$

that is,

$$\left(b^2+2b-1\right)\left(a^4+2a^2+1\right)\geq\left(a^2+2a-1\right)\left(b^4+2b^2+1\right),$$

that is,

$$\left(a^2-b^2\right)\left(a^2b^2-a^2-b^2-3\right)+2(a-b)\left[ab\left(a^2+ab+b^2+2\right)-1\right]\geq 0,$$

which is true as $a\geq b\geq 2$. From (2), we have $h'(y)\geq 0$ for $1\leq y\leq\lfloor\frac{n}{2}\rfloor-1$. Therefore $h(y)$ is an increasing function on $1\leq y\leq\lfloor\frac{n}{2}\rfloor-1$ and hence

$$h(y)\geq h(1)=\frac{(n-2)\,(n-3)}{(n-2)^2+1}+\frac{2}{5}+\frac{2\,(n-2)}{(n-2)^2+4}$$

with equality iff $y=1$. Using this result in (1), we obtain

$$\begin{aligned}\mathrm{ISDD}(\mathrm{DS}_{r,t})&=\frac{(n-t-1)\,(n-t-2)}{(n-t-1)^2+1}+\frac{(t+1)\,t}{(t+1)^2+1}+\frac{(n-t-1)\,(t+1)}{(n-t-1)^2+(t+1)^2}\\&\geq\frac{(n-2)\,(n-3)}{(n-2)^2+1}+\frac{2}{5}+\frac{2\,(n-2)}{(n-2)^2+4}=\mathrm{ISDD}(\mathrm{DS}_{n-3,1}).\end{aligned}$$

Moreover, the equality holds iff $t=1$, that is, iff $T\cong\mathrm{DS}_{n-3,1}$.

Case 2. $d\geq 4$. Let $P_{d+1}:v_1v_2\ldots v_dv_{d+1}$ be a diametral path in tree T. Without loss of generality, we can assume that $d_2\leq d_d$. We have $2\leq d_2\leq\frac{n-1}{2}$. Let $S=\{v_2v_i\in E(T):v_i\in N_T(v_2)\}$. Then $|S|=d_2$. Now,

$$\sum_{\substack{v_i:v_2v_i\in S,\\ d_i=1}}\frac{d_2\,d_i}{d_2^2+d_i^2}=\frac{d_2\,(d_2-1)}{d_2^2+1}\cdot$$

Since $2\leq d_2,\ d_3<n-2$, by Lemma 2.3, we obtain

$$\frac{d_2\,d_3}{d_2^2+d_3^2}>\frac{2\,(n-2)}{(n-2)^2+4}\cdot$$

Let $v_k\in(V(T)\backslash N_T[v_2])\cup\{v_3\}$ be a vertex in T. Then $d_k\leq n-d_2-1$. For any edge $v_iv_j\in E(T)\backslash S$ with $1\leq d_j,\ d_i\leq n-d_2-1$, by Lemma 2.3, we obtain

$$\frac{d_i\,d_j}{d_i^2+d_j^2}\geq\frac{(n-d_2-1)}{(n-d_2-1)^2+1}$$

and hence

$$\sum_{v_iv_j\in E(T)\backslash S}\frac{d_i\,d_j}{d_i^2+d_j^2}\geq\frac{(n-d_2-1)^2}{(n-d_2-1)^2+1}\cdot$$

Now,

$$\begin{aligned}\mathrm{ISDD}(T)&=\sum_{v_iv_j\in E(T)}\frac{d_i\,d_j}{d_i^2+d_j^2}\\&=\sum_{v_iv_j\in E(T)\backslash S}\frac{d_i\,d_j}{d_i^2+d_j^2}+\frac{d_2\,d_3}{d_2^2+d_3^2}+\sum_{\substack{v_i:v_2v_i\in S,\\ d_i=1}}\frac{d_2\,d_i}{d_2^2+d_i^2}\\&>\frac{(n-d_2-1)^2}{(n-d_2-1)^2+1}+\frac{2\,(n-2)}{(n-2)^2+4}+\frac{d_2\,(d_2-1)}{d_2^2+1}\cdot\qquad(3)\end{aligned}$$

Let us consider a function

$$f(y) = \frac{(n-y-1)^2}{(n-y-1)^2+1} + \frac{y\,(y-1)}{y^2+1}, \quad 2 \le y \le \frac{n-1}{2}.$$

Then

$$f'(y) = \frac{y^2+2y-1}{\left(y^2+1\right)^2} - \frac{2\,(n-y-1)}{\left[(n-y-1)^2+1\right]^2} > \frac{y^2+2y-1}{\left(y^2+1\right)^2} - \frac{2}{(n-y-1)^3} > 0,$$

as $2 \le y \le \frac{n-1}{2}$. Therefore $f(y)$ is a strictly increasing function on $2 \le y \le \frac{n-1}{2}$, and hence

$$f(y) \ge f(2) = \frac{(n-3)^2}{(n-3)^2+1} + \frac{2}{5} > \frac{(n-3)\,(n-2)}{(n-2)^2+1} + 0.4$$

as $n \ge d+1 \ge 5$. Using this result in (3), we obtain

$$\mathrm{ISDD}(T) > \frac{(n-3)\,(n-2)}{(n-2)^2+1} + \frac{2\,(n-2)}{(n-2)^2+4} + 0.4 = \mathrm{ISDD}(\mathrm{DS}_{n-3,1}).$$

□

Let $T_{n,i}\,(2 \le i \le n-2)$ be a tree of order n obtained from a path $P_{n-1} : v_1 v_2 \cdots v_i \cdots v_{n-2} v_{n-1}$ by attaching a new pendant edge $v_i v_n$ at v_i. Let $T_{a,b,c}\,(a \ge b \ge c \ge 2,\ a+b+c = n-1)$ be a tree of order n obtained from three paths P_a, P_b and P_c by attaching a new vertex to the exactly one pendant vertex of each of these three paths. We have

$$\mathrm{ISDD}(T_{a,b,c}) = \frac{n-2}{2} + \frac{11}{130}.$$

Theorem 3.2. *Let $T\,(\not\cong P_n)$ be a tree of order $n > 6$. Then $\mathrm{ISDD}(T) \le \frac{n-2}{2} + \frac{11}{130}$ with equality iff $T \cong T_{a,b,c}$.*

Proof. Let Δ be the maximum degree and p be the number of pendant vertices in T. We have $p \ge \Delta \ge 3$ as $T \not\cong P_n$.

Claim 1. For any pendant edge $v_i v_j \in E(T)\,(d_i > d_j)$,

$$\frac{d_i\, d_j}{d_i^2 + d_j^2} \le 0.4 \tag{4}$$

with equality iff $d_i = d_j + 1 = 2$.

Proof of Claim 1. Since $v_i v_j$ is an pendant edge with $d_i > d_j$, we have $d_i \ge 2$ and $d_j = 1$. For $d_i = d_j + 1 = 2$, the equality holds in (4). Otherwise, $d_i \ge 3$. Since $d_j = 1$, we obtain

$$\frac{d_i\, d_j}{d_i^2 + d_j^2} = \frac{d_i}{d_i^2+1} < \frac{1}{d_i} < 0.4$$

as $d_i \ge 3$. This proves the Claim 1. □

If $p \ge 5$, then by Lemma 2.4 with Claim 1, we obtain

$$\mathrm{ISDD}(T) \le \frac{1}{2}\,(n-6) + 5 \times 0.4 = \frac{n-2}{2} < \frac{n-2}{2} + \frac{11}{130} = \mathrm{ISDD}(T_{a,b,c}).$$

Otherwise, $3 \le p \le 4$. We take into account the next two scenarios:

Case 1. $p = 3$. If $T \cong T_{a,b,c}$, then

$$\mathrm{ISDD}(T) = \frac{n-2}{2} + \frac{11}{130}$$

and hence the equality holds. Otherwise, $T \cong T_{n,i}$ $(2 \le i \le n-2)$. For $T \cong T_{n,2}$ (or $T_{n,n-2}$), we obtain

$$\mathrm{ISDD}(T) = \frac{n-5}{2} + 0.4 + 0.3 \times 2 + \frac{6}{13} < \frac{n-2}{2} + \frac{11}{130} = \mathrm{ISDD}(T_{a,b,c}).$$

For $T \cong T_{n,i}$ $(3 \le i \le n-3)$, we obtain

$$\mathrm{ISDD}(T) = \frac{n-6}{2} + 0.4 \times 2 + 0.3 + \frac{6}{13} \times 2 < \frac{n-2}{2} + \frac{11}{130} = \mathrm{ISDD}(T_{a,b,c}).$$

Case 2. $p = 4$. In this case $\Delta \le p = 4$. First we assume that Γ has a pendant edge $v_i v_j \in E(\Gamma)$ with $d_i \ge 3$ and $d_j = 1$. Then $(d_i - 3)(3d_i - 1) \ge 0$, that is, $3d_i^2 + 3 \ge 10d_i$, that is,

$$\frac{d_i\, d_j}{d_i^2 + d_j^2} = \frac{d_i}{d_i^2 + 1} \le 0.3.$$

Using the above result with Claim 1, we obtain

$$\mathrm{ISDD}(T) \le \frac{1}{2}(n-5) + 3 \times 0.4 + 0.3 = \frac{n-2}{2} < \frac{n-2}{2} + \frac{11}{130} = \mathrm{ISDD}(T_{a,b,c}).$$

Next we assume that Γ has all the four pendant edges $v_i v_j \in E(\Gamma)$ such that $(d_i,\, d_j) = (2, 1)$. In this case, there are at least one non-pendant edge $v_i v_j \in E(\Gamma)$ such that $d_i > d_j > 1$. Since $3 \le \Delta \le 4$, by Lemma 2.5, we obtain

$$\frac{d_i\, d_j}{d_i^2 + d_j^2} \le \max\left\{\frac{6}{13}, \frac{12}{25}\right\} = 0.48.$$

Hence

$$\mathrm{ISDD}(T) \le \frac{1}{2}(n-6) + 4 \times 0.4 + 0.48 = \frac{n-2+0.16}{2} < \frac{n-2}{2} + \frac{11}{130} = \mathrm{ISDD}(T_{a,b,c}).$$

□

Remark 3.3. From Theorems 3.1 and 3.2, we conclude that $\mathrm{DS}_{n-3,1}$ gives the second minimum and $T_{a,b,c}$ gives the second maximum inverse symmetric division deg index for all trees of order n.

4. ISDD index of chain graphs

A graph with no induced subgraph isomorphic to C_3, C_5 or $2K_2$ is called a chain graph. In any chain graph Γ of order n, its vertex set consists of two color classes (or co-cliques). Each of these two classes are partitioned into k non-empty cells $U_1, U_2, \ldots, U_k$ and $V_1, V_2, \ldots, V_k$, respectively; all vertices in U_i are joined by (cross) edges to all vertices in $\bigcup_{j=1}^{k+1-i} V_j$ for $i = 1, 2, \ldots, k$. The chain graph is also termed as double nested graph (DNG) [4], difference graph [26], and Ferrers graph [14].

We give an upper bound on $\mathrm{ISDD}(\Gamma)$ in terms of n of chain graphs and the corresponding topological structure of the extremal graph is characterized.

Theorem 4.1. *Let Γ be a chain graph of order n. Then $\mathrm{ISDD}(\Gamma) \le \frac{\lceil \frac{n}{2} \rceil^2 \lfloor \frac{n}{2} \rfloor^2}{\lceil \frac{n}{2} \rceil^2 + \lfloor \frac{n}{2} \rfloor^2}$ with equality iff $\Gamma \cong K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$.*

Proof. We take into account the next two scenarios:

Case 1. $h=1$. In this case $\Gamma \cong K_{r,t}$ $(r+t=n,\ r\geq t)$. From the definition of the inverse symmetric division deg index, we obtain

$$\mathrm{ISDD}(\Gamma)=\frac{r\,t}{r^2+t^2}\,r\,t=\frac{r^2\,t^2}{r^2+t^2}=\frac{(n-t)^2\,t^2}{(n-t)^2+t^2}.$$

Let us consider a function

$$h(y)=\frac{(n-y)^2\,y^2}{(n-y)^2+y^2},\quad y\leq\left\lfloor\frac{n}{2}\right\rfloor.$$

Then we have

$$h'(y)=\frac{2y\,(n-y)\left[(n-y)^3-y^3\right]}{\left[(n-y)^2+y^2\right]^2}.$$

Thus $h(y)$ is an increasing function on $y\leq\frac{n}{2}$ and a decreasing function on $y\geq\frac{n}{2}$. Hence

$$h(y)\leq\max\Big\{h\Big(\left\lceil\frac{n}{2}\right\rceil\Big),\,h\Big(\left\lfloor\frac{n}{2}\right\rfloor\Big)\Big\}=\frac{\left\lceil\frac{n}{2}\right\rceil^2\left\lfloor\frac{n}{2}\right\rfloor^2}{\left\lceil\frac{n}{2}\right\rceil^2+\left\lfloor\frac{n}{2}\right\rfloor^2}$$

with equality iff $y=\lceil\frac{n}{2}\rceil$ or $y=\lfloor\frac{n}{2}\rfloor$.

From the above results, we conclude that $\mathrm{ISDD}(\Gamma)\leq\frac{\lceil\frac{n}{2}\rceil^2\lfloor\frac{n}{2}\rfloor^2}{\lceil\frac{n}{2}\rceil^2+\lfloor\frac{n}{2}\rfloor^2}$ with equality iff $\Gamma\cong K_{\lceil\frac{n}{2}\rceil,\,\lfloor\frac{n}{2}\rfloor}$.

Case 2. $h\geq 2$. Let m be the number of edges in Γ. Since $h\geq 2$, we have $m<\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor$, that is, $m\leq\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor-1$.

First we assume that n is even $(n=2s,$ say). Then by Lemma 2.4, we obtain

$$\frac{d_i d_j}{d_i^2+d_j^2}\leq\frac{1}{2}=\frac{\left\lceil\frac{n}{2}\right\rceil\left\lfloor\frac{n}{2}\right\rfloor}{\left\lceil\frac{n}{2}\right\rceil^2+\left\lfloor\frac{n}{2}\right\rfloor^2}\quad\text{for any edge } v_iv_j\in E(\Gamma)$$

with equality iff $d_i=d_j$. Using these results, one can see easily that

$$\mathrm{ISDD}(\Gamma)=\sum_{v_iv_j\in E(\Gamma)}\frac{d_id_j}{d_i^2+d_j^2}\leq m\,\frac{\left\lceil\frac{n}{2}\right\rceil\left\lfloor\frac{n}{2}\right\rfloor}{\left\lceil\frac{n}{2}\right\rceil^2+\left\lfloor\frac{n}{2}\right\rfloor^2}<\frac{\left\lceil\frac{n}{2}\right\rceil^2\left\lfloor\frac{n}{2}\right\rfloor^2}{\left\lceil\frac{n}{2}\right\rceil^2+\left\lfloor\frac{n}{2}\right\rfloor^2}.$$

Next we assume that n is odd, $n=2s+1$, say. By Lemma 2.4, we obtain

$$\mathrm{ISDD}(\Gamma)=\sum_{v_iv_j\in E(\Gamma)}\frac{d_id_j}{d_i^2+d_j^2}\leq\frac{m}{2}\leq\frac{1}{2}\left(\left\lceil\frac{n}{2}\right\rceil\left\lfloor\frac{n}{2}\right\rfloor-1\right).$$

Now we have to prove that

$$\frac{1}{2}\left(\left\lceil\frac{n}{2}\right\rceil\left\lfloor\frac{n}{2}\right\rfloor-1\right)<\frac{\left\lceil\frac{n}{2}\right\rceil^2\left\lfloor\frac{n}{2}\right\rfloor^2}{\left\lceil\frac{n}{2}\right\rceil^2+\left\lfloor\frac{n}{2}\right\rfloor^2},$$

that is,

$$\frac{1}{2}\left(s\,(s+1)-1\right)<\frac{s^2\,(s+1)^2}{(s+1)^2+s^2},$$

that is,

$$2s^2\,(s+1)^2-s\,(s+1)^3-s^3\,(s+1)+(s+1)^2+s^2>0,$$

that is,

$$s^2+s+1>0,$$

which is always true. Therefore

$$\mathrm{ISDD}(\Gamma) < \frac{\lceil \frac{n}{2} \rceil^2 \lfloor \frac{n}{2} \rfloor^2}{\lceil \frac{n}{2} \rceil^2 + \lfloor \frac{n}{2} \rfloor^2}$$

when n is odd. □

We now obtain a sharp lower bound on ISDD(Γ) in terms of n of chain graphs.

Theorem 4.2. *Let* Γ *be a connected chain graph of order* n*. Then* $\mathrm{ISDD}(\Gamma) \geq \frac{(n-1)^2}{(n-1)^2+1}$ *with equality iff* $\Gamma \cong S_n$*.*

Proof. Let m be the number of edges in chain graphs. Since Γ is connected, $m \geq n-1$. Now, we have to prove that for any edge $v_iv_j \in E(\Gamma)$ $(d_i \geq d_j)$,

$$\frac{d_i\, d_j}{d_i^2 + d_j^2} \geq \frac{(n-1)}{(n-1)^2+1},$$

that is,

$$\frac{d_i}{d_j} + \frac{d_j}{d_i} \leq n - 1 + \frac{1}{n-1},$$

that is,

$$\left(\sqrt{\frac{d_i}{d_j}} - \sqrt{\frac{d_j}{d_i}}\right)^2 \leq \left(\sqrt{n-1} - \frac{1}{\sqrt{n-1}}\right)^2,$$

which is true as $\frac{d_i}{d_j} \leq n-1$, that is, $\sqrt{\frac{d_i}{d_j}} \leq \sqrt{n-1}$ and $\sqrt{\frac{d_j}{d_i}} \geq \frac{1}{\sqrt{n-1}}$, that is,

$$\sqrt{\frac{d_i}{d_j}} - \sqrt{\frac{d_j}{d_i}} \leq \sqrt{n-1} - \frac{1}{\sqrt{n-1}}.$$

Using the above results, we obtain

$$\mathrm{ISDD}(\Gamma) = \sum_{v_iv_j \in E(\Gamma)} \frac{d_id_j}{d_i^2 + d_j^2} \geq \frac{(n-1)}{(n-1)^2+1}\, m \geq \frac{(n-1)^2}{(n-1)^2+1}.$$

Moreover, the above equality holds iff $m = n-1$, and for any edge $v_iv_j \in E(\Gamma)$ $(d_i \geq d_j)$,

$$\frac{d_i\, d_j}{d_i^2 + d_j^2} = \frac{(n-1)}{(n-1)^2+1},$$

that is, iff $\Gamma \cong S_n$. □

5. Upper bound on ISDD index of graphs in terms of order and chromatic number

A k-partite graph is a set of graph vertices that is divided into k disjoint sets such that no two graph vertices from the same set are adjacent. A complete k-partite graph is a k-partite graph where every pair of graph vertices in the k sets are adjacent. If there are n_1, $n_2, \ldots, n_k$ graph vertices in the k sets, the complete k-partite graph is denoted $K_{n_1,n_2,\ldots,n_k}$. The least number of colors required to color a graph's vertices so that no two adjacent vertices have the same color is known as the chromatic number. The Turán graph, denoted by $T(n,k)$, is a complete multipartite graph; it is formed by partitioning a set of n vertices into k subsets, with sizes as equal as possible, and then connecting two vertices by an edge iff they belong to different subsets. If $n = kq+s$, then the Turán graph is of the form $K_{\underbrace{q+1,\ldots,q+1}_{s},\underbrace{q,\ldots,q}_{k-s}}$. Suppose that $H \cong T(kq+s,k) \cong K_{\underbrace{q+1,\ldots,q+1}_{s},\underbrace{q,\ldots,q}_{k-s}}$.

Then

$$V(H) = V_1 \cup V_2 \cup \cdots \cup V_k, \quad V_i \cap V_j = \emptyset\,(i \neq j),$$

and $v_iv_j \in E(H)$, where $v_i \in V_r$, $v_j \in V_t\,(1 \le r \neq t \le k)$. Moreover, $d_i = n-q-1$ for $v_i \in V_r\,(1 \le r \le s)$ and $d_i = n-q$ for $v_i \in V_r\,(s+1 \le r \le k)$. Let S_1, S_2, S_3 be the three set of edges in H defined by

$$\begin{aligned} S_1 &= \{v_iv_j \in E(H) :\, v_i \in V_r,\, v_j \in V_t,\, 1 \le r \neq t \le s\},\\ S_2 &= \{v_iv_j \in E(H) :\, v_i \in V_r,\, v_j \in V_t,\, s+1 \le r \neq t \le k\},\\ \text{and } S_3 &= \{v_iv_j \in E(H) :\, v_i \in V_r,\, v_j \in V_t,\, 1 \le r \le s,\, s+1 \le t \le k\}. \end{aligned}$$

Since the number of edges from the set V_r to the set $V_t\,(1 \le r \neq t \le s)$ in H is $(q+1)^2$. Thus we have

$$|S_1| = \sum_{\substack{v_iv_j \in E(H),\\ v_i \in V_r, v_j \in V_t, 1 \le r \neq t \le s}} 1 = \binom{s}{2}(q+1)^2.$$

Similarly, we obtain

$$|S_2| = \sum_{\substack{v_iv_j \in E(H),\\ v_i \in V_r, v_j \in V_t, s+1 \le r \neq t \le k}} 1 = \binom{k-s}{2} q^2, \quad \text{and} \quad |S_3| = \sum_{\substack{v_iv_j \in E(H),\\ v_i \in V_r, v_j \in V_t, 1 \le r \le s, s+1 \le t \le k}} 1 = s\,(k-s)\,q\,(q+1).$$

Let $m(H)$ be the number of edges in H. Then

$$m(H) = |S_1| + |S_2| + |S_3| = \binom{s}{2}(q+1)^2 + \binom{k-s}{2} q^2 + s\,(k-s)\,q\,(q+1).$$

Now,

$$\begin{aligned} \mathrm{ISDD}(H) &= \sum_{v_iv_j \in E(H)} \frac{d_i\,d_j}{d_i^2 + d_j^2}\\ &= \sum_{\substack{v_iv_j \in E(H),\\ v_i \in V_r, v_j \in V_t, 1 \le r \neq t \le s}} \frac{d_i\,d_j}{d_i^2 + d_j^2} + \sum_{\substack{v_iv_j \in E(H),\\ v_i \in V_r, v_j \in V_t, s+1 \le r \neq t \le k}} \frac{d_i\,d_j}{d_i^2 + d_j^2}\\ &\quad + \sum_{\substack{v_iv_j \in E(H),\\ v_i \in V_r, v_j \in V_t, 1 \le r \le s, s+1 \le t \le k}} \frac{d_i\,d_j}{d_i^2 + d_j^2}\\ &= \sum_{\substack{v_iv_j \in E(H),\\ v_i \in V_r, v_j \in V_t, 1 \le r \neq t \le s}} \frac{1}{2} + \sum_{\substack{v_iv_j \in E(H),\\ v_i \in V_r, v_j \in V_t, s+1 \le r \neq t \le k}} \frac{1}{2}\\ &\quad + \sum_{\substack{v_iv_j \in E(H),\\ v_i \in V_r, v_j \in V_t, 1 \le r \le s, s+1 \le t \le k}} \frac{(n-q-1)\,(n-q)}{(n-q-1)^2 + (n-q)^2}\\ &= \frac{1}{2}\binom{s}{2}(q+1)^2 + \frac{1}{2}\binom{k-s}{2} q^2 + \frac{(n-q)\,(n-q-1)}{(n-q)^2 + (n-q-1)^2}\, s\,(k-s)\,q\,(q+1). \end{aligned} \tag{5}$$

We now present an upper bound on ISDD of graph Γ, and characterize the extremal graphs.

Theorem 5.1. *Let Γ be a graph of order n with chromatic number k. Then*

$$\mathrm{ISDD}(\Gamma) \leq \mathrm{ISDD}(T(n,k))$$

with equality iff $\Gamma \cong T(n,k)$.

Proof. Let $m(\Gamma)$ be the number of edges in Γ. Since Γ has chromatic number k, we have $\Gamma \subseteq K_{n_1,n_2,\ldots,n_k}$, where $n = n_1+n_2+\cdots+n_k$ $(n_1 \geq n_2 \geq \cdots \geq n_k)$. Then $m(\Gamma) \leq m(K_{n_1,n_2,\ldots,n_k})$. Again since Γ has chromatic number k and order n, then there exists a positive integer q such that $n = kq + s$, where $0 \leq s \leq k-1$.

Claim 2. Let $H_1 \cong K_{n_1,n_2,\ldots,n_k}$. Then $m(H_1) \leq \frac{1}{2}\left(1-\frac{1}{k}\right)(n^2-s^2) + \binom{s}{2}$ with equality iff $H_1 \cong T(n,k)$.

Proof of Claim 2. We take into account the next two scenarios:

Case 1. $H_1 \cong T(n,k)$. In this case we can assume that $H_1 \cong K_{\underbrace{q+1,\ldots,\,q+1}_{s},\underbrace{q,\ldots,\,q}_{k-s}}$ and $n = qk+s$, where $0 \leq s < k$. Thus we obtain

$$m(H_1) = \binom{s}{2}(q+1)^2 + \binom{k-s}{2} q^2 + s\,(k-s)\,q\,(q+1).$$

Since $q = \frac{n-s}{k}$, after simplifying from the above result, we obtain

$$m(H_1) = \frac{1}{2}\left(1-\frac{1}{k}\right)(n^2-s^2) + \binom{s}{2}$$

and hence the equality holds.

Case 2. $H_1 \ncong T(n,k)$. In this case there exist two positive integers i and j with $1 \leq i < j \leq k$ such that $n_i - n_j \geq 2$. Then one can easily check that

$$m\big(K_{n_1,\ldots,n_i,\ldots,\,n_j,\ldots,\,n_k}\big) < m\big(K_{n_1,\ldots,n_i-1,\ldots,\,n_j+1,\ldots,\,n_k}\big).$$

Apply the above result several times (if needed), we obtain

$$m(H) = m\big(K_{n_1,\ldots,n_i,\ldots,\,n_j,\ldots,\,n_k}\big) < m\big(K_{n_1,\ldots,n_i-1,\ldots,\,n_j+1,\ldots,\,n_k}\big) < \cdots < m(T(n,k)).$$

This completes the proof of Claim 2.

□

Let $r = \frac{1}{2}\left(1-\frac{1}{k}\right)(n^2-s^2) + \binom{s}{2}$. From (5), we obtain

$$\mathrm{ISDD}(T(n,k)) = \frac{1}{2}\binom{s}{2}(q+1)^2 + \frac{1}{2}\binom{k-s}{2}q^2 + \frac{(n-q)\,(n-q-1)}{(n-q)^2+(n-q-1)^2}\,s\,(k-s)\,q\,(q+1).$$

If $\Gamma \cong T(n,k)$, then $\mathrm{ISDD}(\Gamma) = \mathrm{ISDD}(T(n,k))$ and hence the equality holds. Otherwise, $\Gamma \ncong T(n,k)$. Then by Claim 2, we obtain $m(\Gamma) \leq r-1$. Since

$$\frac{d_\Gamma(v_i)\,d_\Gamma(v_j)}{d_\Gamma(v_i)^2 + d_\Gamma(v_j)^2} \leq \frac{1}{2} \quad \text{for any edge } v_iv_j \in E(\Gamma),$$

we obtain

$$\mathrm{ISDD}(\Gamma) \leq \frac{1}{2}\,m(\Gamma) \leq \frac{1}{2}\,(r-1). \tag{6}$$

We take into account the next two scenarios:

Case 1. $s = 0$. In this case $n = kq$. Using the above results with Lemma 2.4, from the definition of the inverse symmetric division deg index, we obtain

$$\begin{aligned}\mathrm{ISDD}(\Gamma) &= \sum_{v_iv_j \in E(\Gamma)} \frac{d_i d_j}{d_i^2 + d_j^2} \\ &\leq \frac{1}{2}\, m(\Gamma) \leq \frac{1}{2}\,(r-1) = \frac{1}{2}\left[\frac{k(k-1)\,q^2}{2} - 1\right] < \frac{k(k-1)\,q^2}{4} = \mathrm{ISDD}(T(n,k)).\end{aligned}$$

Case 2. $s \geq 1$. Since $s \leq k-1$, $k-1 \geq k-s$ and $2q \geq q+1$, we obtain

$$2q^2\,(k-1)^2 \geq qs\,(q+1)\,(k-s).$$

Since $n = kq + s$, we obtain

$$(q(k-1)+s)^2 + (q(k-1)+s-1)^2 > 2q^2\,(k-1)^2 \geq s\,(k-s)\,q\,(q+1),$$

that is,

$$(n-q)^2 + (n-q-1)^2 > s\,(k-s)\,q\,(q+1),$$

that is,

$$\frac{s\,(k-s)\,q\,(q+1)}{(n-q)^2 + (n-q-1)^2} < 1.$$

Using the above result with (5) and (6), we obtain

$$\begin{aligned}\mathrm{ISDD}(T(n,k)) - \mathrm{ISDD}(\Gamma) &\geq \frac{1}{2}\binom{s}{2}(q+1)^2 + \frac{1}{2}\binom{k-s}{2}q^2 + \frac{(n-q)\,(n-q-1)}{(n-q)^2+(n-q-1)^2} \\ &\quad \times s\,(k-s)\,q\,(q+1) - \frac{1}{2}\,(r-1) \\ &= \frac{1}{2}\left[\binom{s}{2}(q+1)^2 + \binom{k-s}{2}q^2 + s\,(k-s)\,q\,(q+1)\right] \\ &\quad + \left[\frac{(n-q)\,(n-q-1)}{(n-q)^2+(n-q-1)^2} - \frac{1}{2}\right] s\,(k-s)\,q\,(q+1) - \frac{1}{2}\,(r-1) \\ &= \frac{1}{2}\left[\frac{1}{2}\left(1-\frac{1}{k}\right)\left(n^2-s^2\right) + \binom{s}{2}\right] - \frac{1}{2}\,(r-1) \\ &\quad - \left[\frac{1}{2} - \frac{(n-q)\,(n-q-1)}{(n-q)^2+(n-q-1)^2}\right] s\,(k-s)\,q\,(q+1) \\ &= \frac{1}{2} - \frac{s\,(k-s)\,q\,(q+1)}{2\left[(n-q)^2+(n-q-1)^2\right]} > 0.\end{aligned}$$

Hence $\mathrm{ISDD}(T(n,k)) > \mathrm{ISDD}(\Gamma)$. □

6. Concluding remarks

In this letter we determine the second maximal and the second minimal trees with respect to the inverse symmetric division deg index (ISDD). We have established that the star gives the minimal and the complete bipartite graph $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$ gives the maximal graphs with respect to the inverse symmetric division deg index (ISDD) among chain graphs of order n. Finally, we obtained that the Turán graph gives the maximal graph for any graph of order n with chromatic number k.

Future studies on inverse symmetric division deg index (ISDD) might focus on tight bounds for the bicyclic, and tricyclic graphs with identifying extremal graphs.

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References

[1] H. Ahmed, A. Saleh, R. Ismail and A. Alameri, Computational analysis for eccentric neighborhood Zagreb indices and their significance. *Heliyon* **9** (2023) e17998.
[2] A.M. Albalahi and A. Ali, On the inverse symmetric division deg index of unicyclic graphs. *Computation* **10** (2022) 181.
[3] A. Ali, S. Elumalai and T. Mansour, On the symmetric division deg index of molecular graphs. *MATCH Commun. Math. Comput. Chem.* **83** (2020) 205–220.
[4] F.K. Bell, D. Cvetković, P. Rowlinson and S.K. Simić, Graphs for which the least eigenvalue is minimal, I. *Linear Algebra Appl.* **429** (2008) 234–241.
[5] J.A. Bondy and U.S.R. Murty, Graph Theory. Springer (2008).
[6] K.C. Das, Maximizing the sum of the squares of the degrees of a graph. *Discrete Math.* **285** (2004) 57–66.
[7] K.C. Das, On geometric-arithmetic index of graphs. *MATCH Commun. Math. Comput. Chem.* **64** (2010) 619–630.
[8] K.C. Das, On comparing Zagreb indices of graphs. *MATCH Commun. Math. Comput. Chem.* **63** (2010) 433–440.
[9] K.C. Das and S.-G. Lee, On the conjecture of the Estrada index. *Linear Algebra Appl.* **431** (2009) 1351–1359.
[10] K.C. Das, M. Matejić, E. Milovanović and I. Milovanović, Bounds for symmetric division deg index of graphs. *Filomat* **33** (2019) 683–698.
[11] K.C. Das, S.A. Mojallal and S. Sun, On the sum of the k largest eigenvalues of graphs and maximal energy of bipartite graphs. *Linear Algebra Appl.* **569** (2019) 175–194.
[12] K.C. Das, A. Alazemi and M. Andelic, On energy and Laplacian energy of chain graphs. *Discrete Appl. Math.* **284** (2020) 391–400.
[13] Z. Du, B. Zhou and N. Trinajstić, On geometric-arithemetic indices of (molecular) trees, unicyclic graphs and bicyclic graphs. *MATCH Commun. Math. Comput. Chem.* **66** (2011) 681–697.
[14] R. Ehrenborg and S.V. Willigenburg, Enumerative properties of Ferrers graphs. *Discrete Comput. Geom.* **32** (2004) 481–492.
[15] E. Estrada, Characterization of 3D molecular structure. *Chem. Phys. Lett.* **319** (2000) 713–718.
[16] E. Estrada, Atom-bond connectivity and the energetic of branched alkanes. *Chem. Phys. Lett.* **463** (2008) 422–425.
[17] E. Estrada and J.A. Rodríguez-Velázquez, Subgraph centrality in complex networks. *Phys. Rev. E* **71** (2005) 056103.
[18] E. Estrada, L. Torres, L. Rodriguez and I. Gutman, An atom-bond connectivity index: modelling the enthalpy of formation of alkanes. *Indian J. Chem.* **37A** (1998) 849–855.
[19] S. Fajtlowicz, On conjectures of grafti II. *Congr. Numer.* **60** (1987) 189–197.
[20] B. Furtula, A. Graovac and D. Vukičević, Atom-bond connectivity index of trees. *Discrete Appl. Math.* **157** (2009) 2828–2835.
[21] B. Furtula, K.C. Das and I. Gutman, Comparative analysis of symmetric division deg index as potentially useful molecular descriptor. *Int. J. Quantum Chem.* **118** (2018) e25659.
[22] M. Ghorbani, S. Zangi and N. Amraei, New results on symmetric division deg index. *J. Appl. Math. Comput.* **65** (2021) 161–176.
[23] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals, total π-electron energy of alternant hydrocarbons. *Chem. Phys. Lett.* **17** (1972) 535–538.
[24] H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons. *Bull. Chem. Soc. Jpn.* **44** (1971) 2332–2339.
[25] X. Li, Y. Shi and I. Gutman, Graph Energy. Springer, New York (2012).
[26] N.V.R. Mahadev and U.N. Peled, Threshold Graphs and Related Topics. North Holland, New York (1995).
[27] D. Maji and G. Ghorai, Computing F-index, coindex and Zagreb polynomials of the kth generalized transformation graphs. *Heliyon* **6** (2020) e05781.
[28] J. Radon, Über die absolut additiven Mengenfunktionen. *Wiener-Sitzungsber. (IIa)* **122** (1913) 1295–1438.
[29] M. Randić, On characterization of molecular branching. *J. Am. Chem. Soc.* **97** (1975) 6609–6615.
[30] D. Vukičević and M. Gasperov, Bond additive modeling 1. Adriatic indices. *Croat. Chem. Acta* **83** (2010) 243–260.
[31] H. Wiener, Structural determination of paraffin boiling points. *J. Am. Chem. Soc.* **69** (1947) 17–20.
[32] K. Xu, J. Li and Z. Luo, Comparative results between the number of subtrees and Wiener index of graphs. *RAIRO-Oper. Res.* **56** (2022) 2495–2511.