Filomat 32:1 (2018), 165–178
https://doi.org/10.2298/FIL1801165E

Published by Faculty of Sciences and Mathematics,
University of Niš, Serbia
Available at: http://www.pmf.ni.ac.rs/filomat

More on Inverse Degree and Topological Indices of Graphs

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Abstract. The inverse degree of a graph G with no isolated vertices is defined as the sum of reciprocal of vertex degrees of the graph G. In this paper, we obtain several lower and upper bounds on inverse degree $ID(G)$. Moreover, using computational results, we prove our upper bound is strong and has the smallest deviation from the inverse degree $ID(G)$. Next, we compare inverse degree $ID(G)$ with topological indices (Randić index $R(G)$, geometric-arithmetic index $GA(G)$) for chemical trees and also we determine the $n-$vertex chemical trees with the minimum, the second and the third minimum, as well as the second and the third maximum of $ID - R$. In addition, we correct the second and third minimum Randić index chemical trees in [16].

1. Introduction

Through this paper, we consider simple connected graphs. Let $G = (V, E)$ be a graph with $|V| = n$ vertices and $|E| = m$ edges. The degree of a vertex v_i, $1 \leq i \leq n$, of G is the number of edges incident with v_i, and is written $d(v_i)$ such that $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$. In particular, Δ, Δ_2 and δ denote the *maximum*, *second maximum* and the *minimum vertex degree* of G, respectively. A vertex of degree 0 is an *isolated vertex* and a vertex of degree 1 is a *pendant vertex* or *end-vertex*.

Molecular descriptors play a significant role in mathematical chemistry, especially in the QSPR/QSAR investigations. Among them, a special place is reserved for so-called topological indices [10]. Nowadays, there exists a legion of topological indices with some applications in chemistry [20]. Topological indices and graph invariants, based on the degrees, are used for characterizing molecular graphs. Also, topological indices of molecular graphs are one of the oldest and most widely used descriptors in quantitative structure-activity relationships (QSAR). A topological index is a numerical value associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity.

Topological indices based on end-vertex degrees of edges have been used over 40 years. Among them, several indices are recognized to be useful tools in chemical researches. Probably, the best know such

2010 *Mathematics Subject Classification*. Primary 05C07 (mandatory); Secondary 05C35, 05C90 (optionally)
Keywords. First Zagreb index, Second Zagreb index, Inverse degree
Received: 20 February 2017; Accepted: 31 July 2017
Communicated by Paola Bonacini
[b]Research supported by the Science and Engineering Research Board, New Delhi, India. (SERB/F/4168/2012-13)
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descriptor is the Randić connectivity index R [21], which is the most used molecular descriptor in QSPR and QSAR, defined by

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}.$$

In the same time, Gutman and Trinajstić [16] explored the study of total π-electron energy on the molecular structure and introduced two vertex degree-based graph variants $M_1(G)$ and $M_2(G)$. The first and second Zagreb indices are respectively defined by

$$M_1(G) = \sum_{v \in V(G)} d(v)^2 \quad and \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

The Zagreb indices are used by various researchers in their QSPR and QSAR studies, attracting more attention from chemists and mathematicians. For the recent survey see [2] and the references therein.

Motivated by the definition of Randić connectivity index based on the end-vertex degrees of edges in a graph, a new class of topological descriptors, based on some properties of vertices of graph are presented. Vukičević and Furtula [25] introduced the geometric-arithmetic index, which is defined by

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}.$$

Various results on the GA index was reported in the survey [7] and for the recent results we refer [19, 22, 24] and the references cited there in.

The inverse degree appeared first through conjectures of the computer program Graffiti [14]. The inverse degree of a graph G with no isolated vertices is defined by

$$ID(G) = \sum_{v \in V(G)} \frac{1}{d(v)}.$$

It has been studied by many authors in different aspects (see [3, 4, 12]). For recent results and discussions on extremal trees and bounds refer [1, 8, 27].

The paper is organized as follows. In Section 2, we present several lower and upper bounds on inverse degree $ID(G)$ of graph G and which improves the existing bounds of $ID(G)$. In Section 3, we analyze and compare our bounds with existing bounds and we prove that our bounds have the smallest deviation from $ID(G)$. In Section 4, we compare between inverse degree $ID(G)$ with the other topological indices of graphs.

2. Lower Bounds on Inverse degree

In this section, we give some new bounds on inverse degree $ID(G)$ of graph G in terms of n, m, maximum degree Δ, minimal non-pendant degree δ_1, and minimum degree δ. For this we need the following definition. A *biregular graph* is a graph whose vertices have exactly two degrees Δ and δ. Let Γ be the class of graphs such that $d(v_i) = \delta$, $i = 2, 3, \ldots, n$. The class Γ is the special case of the biregular graphs. Let Γ_2 and Γ_3 be the class of graphs, such that $d(v_2) = \cdots = d(v_{n-1}) = \delta$, $d(v_n) = \delta$ with $d(v_1) > d(v_i)$ for $i = 2, 3, \ldots, n$ and $d(v_i) = \delta$ with $d(v_1) \geq d(v_2) > d(v_i)$ for $i = 3, 4, \ldots, n$, respectively.

As usual P_n, $K_{1,n-1}$, C_n denotes the path, star, and cycle graphs on n vertices respectively. A vertex of a graph is said to be pendant if its neighborhood contains exactly one vertex. An edge of a graph is said to be pendant if one of its vertices is a pendant vertex.

Lemma 2.1. (see [11]) *Let a_i and b_i be two sequence of real numbers with $a_i \neq 0$ $(i = 1, 2, \ldots, n)$ and such that $ma_i \leq b_i \leq Ma_i$. Then*

$$\sum_{i=1}^{n} b_i^2 + mM \sum_{i=1}^{n} a_i^2 \leq (M + m) \sum_{i=1}^{n} a_i b_i.$$

Equality holds if and only if either $b_i = ma_i$ or $b_i = Ma_i$ for every $i = 1, 2, \ldots, n$.

Lemma 2.2. (see [8]) *Let G be a graph of order $n > 2$ having m edges and no isolated vertices. Then*

$$ID(G) \geq \frac{\Delta+\delta}{\Delta\delta} + \sqrt{\frac{4(n-2)^3\Delta\delta}{(\Delta+\delta)^2\left[2m(\Delta+\delta) - n\Delta\delta - \Delta^2 - \delta^2\right]}}. \tag{1}$$

Moreover, the equality holds if and only if G is regular.

Lemma 2.3. (see [8]) *Let G be a graph of order $n > 2$ having m edges and no isolated vertices. Then*

$$\frac{\Delta+\delta}{\Delta\delta} + \frac{(n-2)^2}{2m-\Delta-\delta} \leq ID(G) \leq \frac{\Delta+\delta}{\Delta\delta} + \frac{(n-2)\left[(n-3)\left(\Delta^2+\delta^2\right) + 2\Delta\delta\right]}{2\Delta\delta(2m-\Delta-\delta)}. \tag{2}$$

Moreover, the left equality holds in (2) *if and only if $G \in \Gamma_2$ and the right equality holds in* (2) *for regular graphs.*

Now, we give some new improvements in the bounds for the inverse degree of graphs.

Theorem 2.4. *Let G be a simple graph with n vertices, p pendent vertices, m edges, maximum degree Δ and minimal non-pendent vertex degree δ_1. Then*

$$\frac{p\left(\delta_1^2+1\right)}{\Delta^2} + \frac{2(m-p)\delta_1^2}{\Delta^4} \leq ID(G) \leq \frac{p\left(\Delta^2+1\right)}{\delta_1^2} + \frac{2(m-p)\Delta^2}{\delta_1^4}, \tag{3}$$

both the left and right equality holds in (3) *if and only if G is regular graph or biregular graph with $\delta = 1$.*

Proof. For all $uv \in E(G)$, the edge version of the inverse degree of a graph G is

$$ID(G) = \sum_{uv\in E(G)} \frac{d(u)^2 + d(v)^2}{d(u)^2 d(v)^2}.$$

Note that, if there are p pendent edges in the graph G. Then we have

$$\begin{aligned} ID(G) &= \sum_{uv\in E(G), d(v)=1} \frac{d(u)^2+1}{d(u)^2} + \sum_{uv\in E(G), d(v)>1} \frac{d(u)^2+d(v)^2}{d(u)^2d(v)^2} \leq p\frac{\left(\Delta^2+1\right)}{\delta_1^2} + \sum_{uv\in E(G), d(v)>1, d(u)\leq\Delta} \frac{d(u)^2+d(v)^2}{d(u)^2d(v)^2}, \\ &\leq \frac{p\left(\Delta^2+1\right)}{\delta_1^2} + \frac{2(m-p)\Delta^2}{\delta_1^4}, \quad \text{as } \delta_1 \leq d(u), d(v) \leq \Delta. \end{aligned}$$

Now suppose that the equality holds in (3). Then all inequalities in the above argument must be equalities. Therefore, we have $d(u) = \Delta$ and $d(v) = 1$ for each pendent edge $uv \in E(G)$, and $d(u) = \Delta$ for each non-pendent vertex $u \in V(G)$. Suppose that $m = p$, then G is the star $K_{1,n-1}$. Suppose that $m > p$. at first, for $p = 0$, i.e., there is no pendent vertex in G, then we have $d(u) = \Delta$ for every $u \in V(G)$. Thus, G is a regular graph. If $p > 0$, in this case we have $d(u) = \Delta$ for each non-pendent vertex $u \in V(G)$. Hence, G is a biregular graph with $\delta = 1$.

Conversely, one can easily examine that the equality holds in (3) for the $K_{1,n-1}$ or a regular graph or a biregular graph with $\delta = 1$. The left inequality also attained by the above arguments. This completes the proof. □

The *pineapple graph* K_p^q is obtained by appending q pendant edges to a vertex of a complete graph K_p, where $q \geq 1$ and $p \geq 3$.

Remark 2.5. *It is interesting to see that for K_p^3 with $p < 9$ the upper bound in* (2) *is better than the upper bound in* (3) *and for $p \geq 9$,* (3) *is better than* (2). *It is easy to see that the lower bound in* (1) *and* (2) *is stronger than the lower bound* (3) *other than its equality cases.*

Next, we are indeed to improve the lower bound in (2), for which we need the following lemma.

Lemma 2.6. (see [5]) *Let G be a graph with n vertices and m edges . Then*

$$M_1(G) \geq \Delta^2 + \delta^2 + \frac{(2m - \Delta - \delta)^2}{n-2},$$

equality holds if and only if $G \in \Gamma_2$.

Theorem 2.7. *Let G be a simple graph of order* $n(\geq 3)$ *with no isolated vertices. Then*

$$ID(G) \geq \frac{\Delta + \delta}{\Delta\delta} + \frac{(n-2)(2m - \Delta - \delta)}{M_1(G) - \Delta^2 - \delta^2}, \tag{4}$$

equality holds if and only if $G \in \Gamma_2$.

Proof. Let a_i, b_i, c_i and d_i, $i = 1, 2, \ldots, r$, are the sequence of real numbers and x_i, y_i be the non-negative weights. Let $\alpha, \beta \in \mathbb{R}$ then, we start our proof with Root Mean Square - Geometric Mean inequality that $\alpha^2 + \beta^2 \geq 2\alpha\beta$ and equality holds for $\alpha = \beta$. So we get

$$a_i^2 b_j^2 + c_i^2 d_j^2 \geq 2a_i b_j c_i d_j.$$

Multiplying the non-negative weights x_i, y_j and summing over i, j we have

$$\sum_{i=1}^{r}\sum_{j=1}^{r}\left[x_i y_j a_i^2 b_j^2 + x_i y_j c_i^2 d_j^2\right] \geq 2\sum_{i=1}^{r}\sum_{j=1}^{r}\left[x_i y_j a_i b_j c_i d_j\right],$$

which implies

$$\sum_{i=1}^{r} x_i a_i^2 \sum_{i=1}^{r} y_i b_i^2 + \sum_{i=1}^{r} x_i c_i^2 \sum_{i=1}^{r} y_i d_i^2 \geq 2\left(\sum_{j=1}^{r} x_i a_i c_i \sum_{i=1}^{r} y_i b_i d_i\right).$$

If we set $r = n-2$, $a_i = d_i = d(v_{i+1})$, $b_i = c_i = 1$, $i = 1, 2, \ldots, r$, $x_i = \dfrac{1}{d(v_{i+1})}$, $y_i = 1$ in the above, we get

$$(n-2)\sum_{i=2}^{n-1} d(v_i) + \sum_{i=2}^{n-1}\frac{1}{d(v_i)}\sum_{i=2}^{n-1} d(v_i)^2 \geq 2(n-2)\sum_{i=2}^{n-1} d(v_i).$$

Since $\sum_{i=2}^{n-1}\frac{1}{d(v_i)} = ID(G) - \frac{1}{\Delta} - \frac{1}{\delta}$, we have

$$\left(M_1(G) - \Delta^2 - \delta^2\right)\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\delta}\right) \geq (n-2)(2m - \Delta - \delta).$$

Suppose that the equality holds in (4) along with the equality of Lemma 2.6, we get

$$(2m - \Delta - \delta)\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\delta}\right) = (n-2)^2$$

Case (i) For $n = 2$

$$\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\delta}\right) = (n-2) \text{ and } (2m - \Delta - \delta) = (n-2)$$

holds if G is a P_2.
Case (ii) For $n > 2$, the only chance is

$$\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\delta}\right) = \frac{(n-2)}{d(v_i)} \text{ and } (2m - \Delta - \delta) = (n-2)d(v_i),$$

which is possible if $d(v_2) = d(v_3) = \cdots = d(v_{n-1})$. Hence, $G \in \Gamma_2$.

Conversely, if $G \in \Gamma_2$, then $2m - \Delta - \delta = (n-2)\delta$ and $M_1(G) = \Delta^2 + \delta^2 + (n-2)\delta^2$, so we get

$$\frac{(n-2)(2m - \Delta - \delta)}{M_1(G) - \Delta^2 - \delta^2} = (n-2)\frac{1}{\delta}$$
$$\frac{1}{\Delta} + \frac{1}{\delta} + \frac{(n-2)(2m - \Delta - \delta)}{M_1(G) - \Delta^2 - \delta^2} = ID(G),$$

as required. □

Corollary 2.8. *With the assumptions in Theorem 2.7, one has the inequality*

$$ID(G) \geq \frac{\Delta + \Delta_2}{\Delta\Delta_2} + \frac{(2m - \Delta - \Delta_2)(n-2)}{M_1(G) - \Delta^2 - {\Delta_2}^2}, \tag{5}$$

equality holds if and only if $G \in \Gamma_3$.

Remark 2.9. *The lower bounds* (2) *and* (5) *are incomparable. Namely, there exist a molecular graph 1,1,2,2-Tetramethylcyclopropane* (5) *is better than* (2) *and for 1,1,2,3-Tetramethylcyclopropane,* (2) *is better than* (5). *It is easy to see that, the lower bound in Theorem 2.7 is stronger than Lemma 2.2. But, still the lower bound in Lemma 2.3 is stronger than lower bound in Theorem 2.7.*

Theorem 2.10. *Let G be a simple graph of order $n > 2$ with no isolated vertices. Then*

$$n + \frac{M_1(G) - (2m-n)(\Delta+\delta) - 2m}{\Delta\delta} \leq ID(G) \leq \frac{n(\Delta+\delta) - 2m}{\Delta\delta}. \tag{6}$$

Moreover, both the left and right equality holds in (6) *if and only if G is regular or biregular.*

Proof. Let w_i, $i = 1, 2, \ldots, n$, be a sequence of non negative real numbers. Then the weighted version of the Diaz-Metcalf inequality can be expressed as

$$\sum_{i=1}^{n} w_i b_i^2 + mM \sum_{i=1}^{n} w_i a_i^2 \leq (M+m) \sum_{i=1}^{n} w_i a_i b_i. \tag{7}$$

Setting $w_i = \dfrac{1}{d(v_i)}$, $a_i = d(v_i)$, $b_i = 1$, $M = \dfrac{1}{\delta}$ and $m = \dfrac{1}{\Delta}$ for $i = 1, 2, \ldots, n$; by (7) we have

$$\sum_{i=1}^{n} \frac{1}{d(v_i)} + \frac{1}{\Delta\delta} \sum_{i=1}^{n} d(v_i) \leq \left(\frac{1}{\delta} + \frac{1}{\Delta}\right) \sum_{i=1}^{n} 1,$$

which leads to

$$\sum_{i=1}^{n} \frac{1}{d(v_i)} \leq \left(\frac{\Delta+\delta}{\Delta\delta}\right) \sum_{i=1}^{n} 1 - \frac{1}{\Delta\delta} \sum_{i=1}^{n} d(v_i).$$

Thus,

$$ID(G) \leq n\left(\frac{\Delta+\delta}{\Delta\delta}\right) - \frac{2m}{\Delta\delta}.$$

Now, by fixing $w_i = 1 - \frac{1}{d(v_i)}$, $a_i = 1$, $b_i = d(v_i)$, $M = \Delta$ and $m = \delta$, $i = 1, 2, \ldots, n$ in (7), we have

$$\sum_{i=1}^{n} d(v_i)^2 - \sum_{i=1}^{n} d(v_i) + \Delta\delta\left(\sum_{i=1}^{n} 1 - \sum_{i=1}^{n} \frac{1}{d(v_i)}\right) \leq (\Delta + \delta)\left(\sum_{i=1}^{n} d(v_i) - \sum_{i=1}^{n} 1\right).$$

From the above, we get

$$\Delta\delta \sum_{i=1}^{n} \frac{1}{d(v_i)} \geq \Delta\delta \sum_{i=1}^{n} 1 + \sum_{i=1}^{n} d(v_i)^2 - \sum_{i=1}^{n} d(v_i) + \sum_{i=1}^{n} 1 - (\Delta + \delta)\left(\sum_{i=1}^{n} d(v_i) - \sum_{i=1}^{n} 1\right),$$

which implies

$$ID(G) = \sum_{i=1}^{n} \frac{1}{d(v_i)} \geq n + \frac{M_1(G) - (2m - n)(\Delta + \delta) - 2m}{\Delta\delta},$$

as claimed. □

Remark 2.11. *It is clear that the upper bound in* (6) *is stronger than the upper bound in* (2)*. But still the lower bounds in* (6) *and* (2) *are incomparable. For example, there exists a molecular graph 1,1,2-Trimethylcyclobutane for which* (6) *is better than* (2) *and for the molecular graph 1,2,3-Trimethylcyclobutane for which* (2) *is better than* (6)*.*

Theorem 2.12. *Let G be a simple graph of order $n > 2$ with m edges and no isolated vertices, with a vertices of maximum degree Δ and b vertices of degree δ. Then*

$$ID(G) \leq \left(\frac{a}{\Delta} + \frac{b}{\delta}\right) + \frac{(n - b)\Delta + (n - a)\delta - 2m}{(\Delta - 1)(\delta + 1)}, \tag{8}$$

equality holds if and only if the vertex degrees are equal to δ, $\delta + 1$, $\Delta - 1$ or Δ.

Proof. Let $a, A \in \mathbb{R}$ and x_i, y_i be two sequences of real numbers with the property $ay_i \leq x_i \leq Ay_i$ for $i = 1, 2, \ldots, n$ and w_i be any sequence of positive real numbers, we have $w_i (Ay_i - x_i)(x_i - ay_i) \geq 0$. Since w_i is a positive sequence, by choosing $w_i = \frac{1}{d(v_i)}$, $x_i = d(v_i)$, $y_i = 1$, $A = \Delta$ and $a = \delta$, we have

$$\frac{1}{d(v_i)} (\Delta - d(v_i))(d(v_i) - \delta) \geq 0$$

and adding over the vertices by restricting $\delta < d(v_i) < \Delta$, it holds

$$\sum_{\delta < d(v_i) < \Delta} \frac{1}{d(v_i)} (\Delta - d(v_i))(d(v_i) - \delta) \geq \sum_{\delta < d(v_i) < \Delta} \frac{1}{d(v_i)} (\Delta - \delta - 1) \geq 0,$$

which gives

$$\sum_{\delta < d(v_i) < \Delta} \left((\Delta + \delta) - \frac{\Delta\delta}{d(v_i)} - d(v_i)\right) \geq (\Delta - \delta - 1) \sum_{\delta < d(v_i) < \Delta} \frac{1}{d(v_i)}.$$

Expanding the above inequality gives the required result with equality if and only if $d(v_i) = \delta + 1$ or $d(v_i) = \Delta - 1$, which completes the proof. □

Corollary 2.13. *Let T be a tree of order $n > 2$ with no isolated vertices out of which a vertices of maximum degree Δ and b vertices of degree δ. Then*

$$ID(T) \leq \left(\frac{a}{\Delta} + \frac{b}{\delta}\right) + \frac{(n - b)\Delta + (n - a)\delta - 2(n - 1)}{(\Delta - 1)(\delta + 1)}, \tag{9}$$

equality holds if and only if the vertex degrees are equal to δ, $\delta + 1$, $\Delta - 1$ or Δ.

Lemma 2.14. *Let T be a tree on n vertices, then*

$$\frac{n+2}{2} \leq ID(T) \leq (n-1) + \frac{1}{n-1}, \tag{10}$$

where the lower and upper bounds are attained if and only if $T = P_n$ and $T = K_{1,n-1}$ respectively.

It is easy to see that the upper bound in (9) is always better than (10).

3. Computational Results

In this section, we compare the upper bounds for inverse degree. In Table 2 and Table 3, we present the computational results for connected graphs on $n = 3$ to $n = 9$ vertices and connected trees on n = 10 to 20 vertices respectively. In the group one of the Table 1 and Table 2, the first column represents the degree of the vertex n,the second column contains number of connected graphs (trees) on n vertices and the third one has the average value of the inverse degree $ID(G)$. Next two groups of three columns represent the average value of the upper bound, the standard deviation $\sqrt{\frac{\sum_G (X(G)-ID(G))^2}{count}}$ and the number of graphs for which the equality holds.

Parameters			Lemma 2.3			Theorem 2.10			Theorem 2.12		
n	Count	Avg.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.
3	2	2.0000	2.0000	0.0000	2	2.0000	0.0000	2	2.0000	0.0000	2
4	6	2.2778	2.4444	0.3043	4	2.3333	0.1361	5	2.2778	0.0000	6
5	21	2.4643	2.8820	0.6790	2	2.6230	0.2709	11	2.4643	0.0000	21
6	112	2.6170	3.2714	0.9857	5	2.9013	0.4364	36	2.6222	0.0243	106
7	853	2.6970	3.6115	1.2679	4	3.1245	0.6078	91	2.7155	0.0510	683
8	11117	2.7050	3.8075	1.4984	17	3.2374	0.7482	471	2.7453	0.0855	6658
9	261080	2.6583	3.8651	1.6527	22	3.2484	0.8366	2296	2.7236	0.1215	105659

Table 1: Upper Bound Comparison on $ID(G)$ for small graphs

Parameters			Lemma 2.3			Theorem 2.10			Theorem 2.12		
n	Count	Avg.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.
10	106	7.2067	11.7949	5.8694	0	7.9146	0.7736	5	7.2146	0.0218	91
11	235	7.8667	13.2310	6.6845	0	8.7339	0.9306	3	7.8790	0.0296	189
12	551	8.5274	14.5902	7.4093	0	9.5370	1.0763	5	8.5450	0.0383	413
13	1301	9.1855	16.0099	8.1819	0	10.3525	1.2348	2	9.2091	0.0476	913
14	3159	9.8457	17.4180	8.9423	0	11.1646	1.3894	10	9.8759	0.0574	2075
15	7741	10.5052	18.8657	9.7421	0	11.9841	1.5508	2	10.5426	0.0678	4774
16	19320	11.1654	20.3115	10.5453	0	12.8022	1.7109	9	11.2105	0.0786	11214
17	48629	11.8256	21.7838	11.3773	0	13.6250	1.8748	6	11.8791	0.0898	26619
18	123867	12.4862	23.2626	12.2202	0	14.4479	2.0388	16	12.5485	0.1015	64057
19	317955	13.1470	24.7585	13.0825	0	15.2735	2.2049	2	13.2186	0.1135	155575
20	823065	13.8080	26.2636	13.9568	0	16.0999	2.3717	27	13.8893	0.1259	381521

Table 2: Upper Bound Comparison on $ID(G)$ for small trees

4. Inverse Degree of Chemical Graphs

A *chemical graph* is a labeled graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds with the maximum degree at most four. Let G be a chemical graph of order $n \geq 3$ and m edges with $n - 1 \leq m \leq 2n$. For integers i and j with $1 \leq i \leq j \leq 4$, an ij-edge means an edge that connects vertices of degree i and j, denote by m_{ij} the number of ij-edges of G. Then

$$ID(G) = \frac{5}{4}m_{12} + \frac{10}{9}m_{13} + \frac{17}{16}m_{14} + \frac{1}{2}m_{22} + \frac{13}{36}m_{23} + \frac{5}{16}m_{24} + \frac{2}{9}m_{33} + \frac{25}{144}m_{34} + \frac{1}{8}m_{44}$$

From the results obtained in [15], we have

$$m_{14} = \frac{4n-2m}{3} - \frac{4}{3}m_{12} - \frac{10}{9}m_{13} - \frac{2}{3}m_{22} - \frac{4}{9}m_{23} - \frac{1}{3}m_{24} - \frac{2}{9}m_{33} - \frac{1}{9}m_{34}$$
$$m_{44} = \frac{5m-4n}{3} + \frac{1}{3}m_{12} + \frac{1}{9}m_{13} - \frac{1}{3}m_{22} - \frac{5}{9}m_{23} - \frac{2}{3}m_{24} - \frac{7}{9}m_{33} - \frac{8}{9}m_{34}.$$

Thus,

$$ID(G) = \left(\frac{15}{12}n - \frac{1}{2}m\right) - \frac{1}{8}m_{12} - \frac{1}{18}m_{13} - \frac{1}{4}m_{22} - \frac{13}{72}m_{23} - \frac{1}{8}m_{24} - \frac{1}{9}m_{33} - \frac{1}{8}m_{34} \tag{11}$$

with negative coefficients for $m_{12}, m_{13}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}$. Also in [15] deduced

$$m_{12} = 2n - 3m - \frac{2}{3}m_{13} - \frac{1}{2}m_{14} + \frac{1}{3}m_{23} + \frac{1}{2}m_{24} + \frac{2}{3}m_{33} + \frac{5}{6}m_{34} + m_{44}$$
$$m_{22} = 3m - 2n - \frac{1}{3}m_{13} - \frac{1}{2}m_{14} - \frac{4}{3}m_{23} - \frac{3}{2}m_{24} - \frac{5}{3}m_{33} - \frac{11}{6}m_{34} - 2m_{44},$$

and then we have

$$ID(G) = \left(\frac{3}{2}n - m\right) + \frac{1}{9}m_{13} + \frac{5}{8}m_{14} + \frac{9}{16}m_{23} + \frac{3}{16}m_{24} + \frac{2}{9}m_{33} + \frac{43}{144}m_{34} + \frac{1}{4}m_{44} \tag{12}$$

with positive coefficients for $m_{13}, m_{14}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}$. From (11) and (12), we have:

Theorem 4.1. *Let G be a chemical graph with $n \geq 3$ vertices and m edges with $n - 1 \leq m \leq 2n$. Then*

$$\frac{3}{2}n - m \leq ID(G) \leq \frac{15}{12}n - \frac{1}{2}m$$

with left equality holds if and if G is either a path or a cycle, and with right equality holds if and only if G has only vertices of degree one and four or 4-regular.

Taking into the account of chemical trees, we have the following corollary.

Corollary 4.2. *Let T be a chemical tree with $n \geq 3$ vertices, then*

$$\frac{n+2}{2} \leq ID(T) \leq \frac{3n+2}{4}, \tag{13}$$

with left equality holds if and only if T is a path, and the right equality holds if and only if T has only vertices of degree one and four.

The left inequality in (13) is also proved in [1] for the case of trees.

Remark 4.3. *By direct comparison of the upper bounds in* (13) *and* (10) *for the chemical trees, we conclude that* (13) *is always better than* (10).

5. Comparison between inverse degree and other topological indices of graphs

In this section we compare inverse degree $ID(G)$ with topological indices (R- index, GA-index) of graphs. We start with an example.

Example 5.1. *For a path P_n, $R(P_n) = \frac{n-3}{2} + \sqrt{2} < \frac{n+2}{2} = ID(P_n)$. For a complete graph K_n, $R(K_n) = \frac{n}{2} > \frac{n}{(n-1)} = ID(K_n)$. For a cycle C_n, the inverse degree coincides with R.*

Table 3: Values of $\frac{1}{\sqrt{d(u)d(v)}}$, $\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$ and $\frac{d(u)^2+d(v)^2}{d(u)^2d(v)^2}$ for all possible degree pairs in chemical tree

$(d(u), d(v))$	$(4,1)$	$(4,2)$	$(4,3)$	$(4,4)$	$(3,1)$	$(3,2)$	$(3,3)$	$(2,1)$	$(2,2)$
$\frac{1}{\sqrt{d(u)d(v)}}$	$\frac{1}{2}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{3}}$	$\frac{1}{4}$	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{3}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2}$
$\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$	$\frac{4}{5}$	$\sqrt{\frac{8}{9}}$	$\sqrt{\frac{48}{49}}$	1	$\sqrt{\frac{3}{4}}$	$\sqrt{\frac{24}{25}}$	1	$\sqrt{\frac{8}{9}}$	1
$\frac{d(u)^2+d(v)^2}{d(u)^2d(v)^2}$	$\frac{17}{16}$	$\frac{5}{16}$	$\frac{25}{144}$	$\frac{1}{8}$	$\frac{10}{9}$	$\frac{13}{36}$	$\frac{2}{9}$	$\frac{5}{4}$	$\frac{1}{2}$

This concludes $ID(G)$ and $R(G)$ incomparable. At first we start with the chemical trees.

Theorem 5.2. *Let T be a chemical tree of order n with no isolated vertices, then $ID(T) > R(T)$.*

Proof. If $n = 2$, then T is isomorphic to $K_{1,1}$ and hence $ID(T) > R(T)$. Since T is a chemical tree, we must have $1 \le d(u), d(v) \le 4$. Thus we have the edges with possible degree pairs

$$(4,1), (4,2), (4,3), (4,4), (3,1), (3,2), (3,3), (2,1), (2,2).$$

In Table 1, we calculate the values of $\frac{1}{\sqrt{d(u)d(v)}}$ and $\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$ for all above degree pairs. From Table 3, one can see easily that

$$\frac{d(u)^2+d(v)^2}{d(u)^2d(v)^2} - \frac{1}{\sqrt{d(u)d(v)}} = \begin{cases} \ge 0.5337 & for\ (d(u),d(v)) = (4,1),(3,1),(2,1), \\ = 0 & for\ (d(u),d(v)) = (2,2), \\ \ge -0.125 & for\ (d(u),d(v)) = (4,4),(4,3),(4,2),(3,3),(3,2). \end{cases} \tag{14}$$

Let a be the number of non-pendent edges in T. Then we have $a+1$ non-pendent and $n-1-a$ pendent vertices in T. Thus,

$$\begin{aligned} ID(T) - R(T) &= \sum_{uv\in E}\left(\frac{d(u)^2+d(v)^2}{d(u)^2d(v)^2} - \frac{1}{\sqrt{d(u)d(v)}}\right) \\ &= \sum_{uv\in E, d(v)=1}\left(\frac{d(u)^2+d(v)^2}{d(u)^2d(v)^2} - \frac{1}{\sqrt{d(u)d(v)}}\right) + \sum_{uv\in E, d(v)\neq 1}\left(\frac{d(u)^2+d(v)^2}{d(u)^2d(v)^2} - \frac{1}{\sqrt{d(u)d(v)}}\right) \\ &\ge (n-1-a)\left(\frac{10}{9} - \frac{1}{\sqrt{3}}\right) - a\left(\frac{1}{8}\right) > 0, \end{aligned}$$

which concludes the Theorem. □

In [18], among the n-vertex chemical trees, the minimum (maximum), the second and third minimum (maximum) for the Randić index is calculated. Now we give the extremal trees for the trees. For the non-pendent edge $(2,2)$, we have $ID - R$ is zero, which leads to the following results.

Theorem 5.3. *Let T be a tree of order n. Then*

(a) *for $n \ge 5$, the ones with only degrees one and two are the unique trees with minimum $ID - R$, which is equal to $2\left(\frac{5}{4} - \frac{1}{\sqrt{2}}\right)$;*

(b) *for $n \ge 7$, the ones with a single vertex of degree three adjacent to three vertices of degree two, and without vertices of degree four are the unique trees with the second minimum $ID - R$, which is equal to $3\left(\frac{5}{4} - \frac{1}{\sqrt{2}}\right) + 3\left(\frac{13}{36} - \frac{1}{\sqrt{6}}\right)$;*

(c) *for $n \geq 6$, the ones with a single vertex of degree three adjacent to two vertices of degree two and one vertex of degree one, and without vertices of degree four are the unique trees with the third minimum ID − R, which is equal to* $2\left(\frac{5}{4}-\frac{1}{\sqrt{2}}\right)+2\left(\frac{13}{36}-\frac{1}{\sqrt{6}}\right)+\left(\frac{10}{9}-\frac{1}{\sqrt{3}}\right)$;

In [18], the general formula for the second and third minimum R index is obtained for chemical trees of order $n \equiv 2(\text{mod } 3) \geq 17$ and $n \equiv 1(\text{mod } 3) \geq 13$ respectively. In addition, Figs. 1 and 2 represents the small n vertex chemical trees for $6 \leq n \leq 24$.

Remark 5.4. *The conclusion which relates to the second and third minimal chemical tree for $n = 11$ and $n = 14$ are wrong. In [18], the second and third minimum R index tree of order 11 is depicted as T_{11}^7 and T_{11}^2. But the trees T_{11}^2 and T_{11}^3 posses the second and third minimum R for order 11. Next, the third minimum R index of order 14 is given as T_{14}^8. But actually it is eighth minimum, the correct tree is T_{14}^3 given in Fig.1.*

Theorem 5.5. *Let T be a chemical tree of order n. Then*

(i) *If $n \equiv 2(\text{mod}3)$, then among the $n-$vertex chemical trees,*
  (a) *for $n \geq 5$, the ones with only degrees one and four are the unique trees with the maximum ID − R.*
  (b) *for $n \geq 17$, the ones with a single vertex of degree two adjacent to two vertices of degree four and a single vertex of degree three adjacent to three vertices of degree four, with second maximum ID − R.*
  (c) *for $n \geq 17$, the ones with a single vertex of degree two and degree three, such that they are adjacent to each other and the remaining adjacent vertices are of degree four, has third maximum ID − R.*

(ii) *If $n \equiv 1(\text{mod}3)$, then among the $n-$vertex chemical trees,*
  (a) *for $n \geq 13$, the ones with a single vertex of degree three adjacent to three vertices of degree four, and without vertices of degree two, with maximum ID − R.*
  (b) *for $n \geq 13$, the ones with a single vertex of degree three adjacent to a vertex of degree one and two vertices of degree four, and without vertices of degree two, with second maximum ID − R.*
  (c) *for $n \geq 13$, the ones with a single vertex of degree three adjacent to a vertex of degree four and two vertices of degree one, with third maximum ID − R.*

(iii) *If $n \equiv 0(\text{mod}3)$, then among the $n-$vertex chemical trees,*
  (a) *for $n \geq 9$, the ones with a single vertex of degree two adjacent to two vertices of degree four, and without vertices of degree three, with maximum ID − R.*
  (b) *for $n \geq 9$, the ones with a single vertex of degree two adjacent to a vertex of degree four and degree one, and without vertices of degree three, with second maximum ID − R.*
  (c) *for $n \geq 18$, the ones with two vertices of degree three adjacent to three vertices of degree four, and without vertices of degree two, with third maximum ID − R.*

In [8], the following results on the comparison between $ID(G)$ with $GA(G)$ presented.

Lemma 5.6. (see [8]) *Let G be a graph with no isolated vertices, maximum degree Δ, and minimum degree δ. If the average degree $\overline{d} \geq 2\sqrt{\frac{\Delta}{\delta^3}}$, then $GA(G) \geq ID(G)$.*

For any simple graph G of order n and m edges, the average degree $\overline{d}$ is defined by $\overline{d} = \frac{2m}{n}$.
If G is a acyclic graph, then the minimum degree $\delta = 1$, maximum degree $2 \leq \Delta \leq n-1$ and $\overline{d} = 2\left(1-\frac{1}{n}\right)$.
Comparing Theorem 5.6 with the above results, we get $2\left(1-\frac{1}{n}\right) < 2\sqrt{2}$. This concludes that the family of trees are totally eliminated due to the assumption in the Theorem 5.6.

Example 5.7. *For a path $P_n(> 4)$, $GA(P_n) = n - 3 + \frac{4\sqrt{2}}{3} > \frac{n+2}{2} = ID(P_n)$. For a star $K_{1,n-1}$, $GA(K_{1,n-1}) = \frac{2(n-1)^{\frac{3}{2}}}{n} < (n-1) + \frac{1}{(n-1)} = ID(K_{1,n-1})$.*

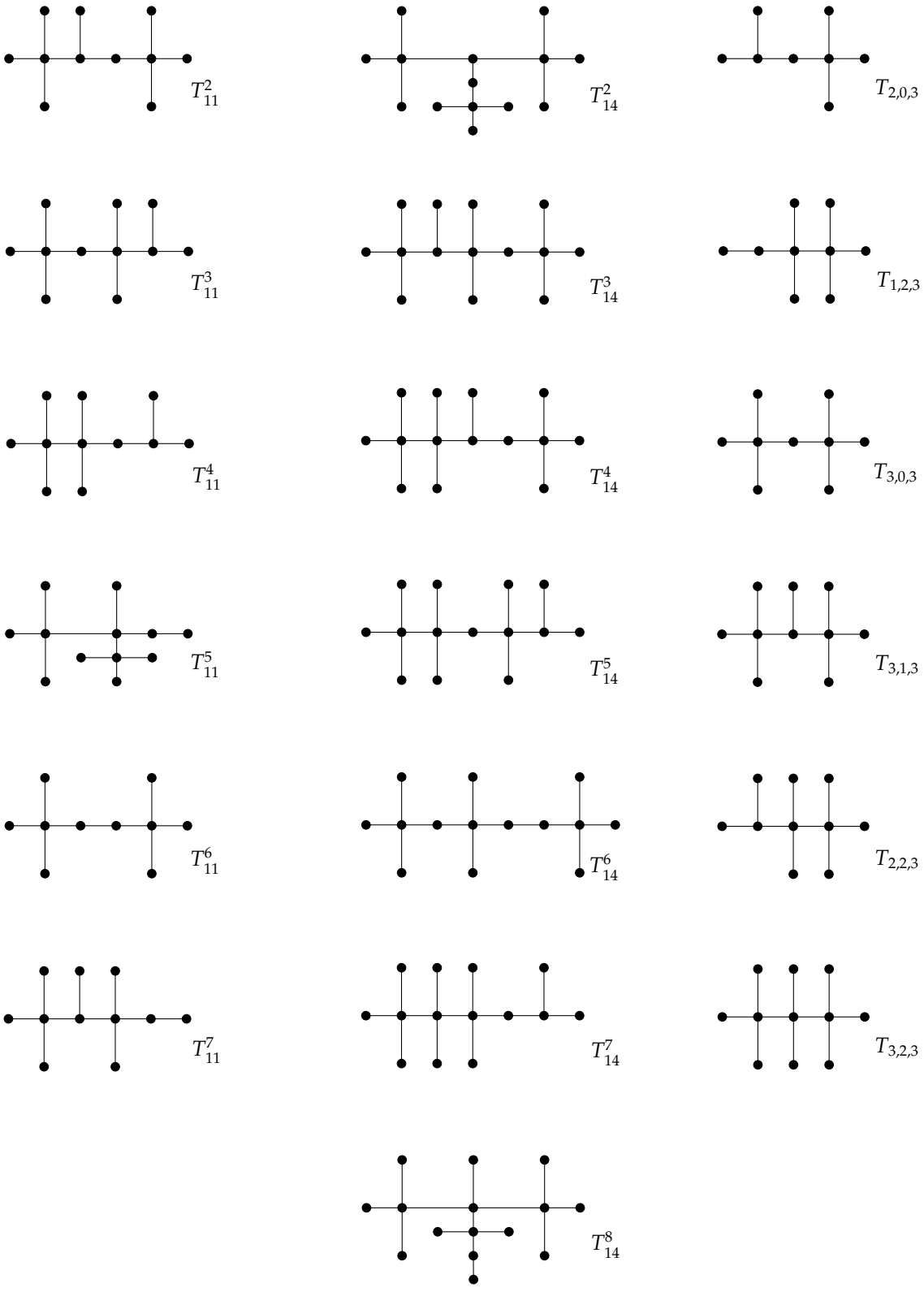

Figure 1: Chemical trees on 11 vertices (left) and 14 vertices (middle) with second to seventh and second to eigth minimal (if the minimal trees are not unique, one representative is shown) Randić index. Chemical trees (right) between 8 to 11 vertices with $ID(T) > GA(T)$.

This concludes, inverse degree and GA index are incomparable for trees. Now we compare inverse degree with GA index of trees.

Let G and H be graphs. We denote by $\sigma_G(H)$ the number of distinct subgraphs of the graph G which are isomorphic to H. Let α, β and γ be whole numbers. $T_{\alpha,\beta}$ and $T_{\alpha,\gamma,\beta}$ are the double and triple star trees on $\alpha+\beta+2$, $\alpha+\gamma+\beta+3$ vertices respectively. $T_{\alpha,\beta}$ is obtained from P_2, by attaching α pendent vertices to its one of the vertex and β pendent vertices to its other vertex. $T_{\alpha,\gamma,\beta}$ is obtained from P_3, by attaching α, β pendent vertices to its end vertices and γ pendent vertices to its middle vertex. Obviously $T_{0,0} \equiv P_2, T_{1,0} \equiv P_3$ and $T_{n-2,0} \equiv T_{0,n-2} \equiv K_{1,n-1}$.

Theorem 5.8. *Let T be a $T_{\alpha,\beta}$ double star. Then $ID(T_{\alpha,\beta}) > GA(T_{\alpha,\beta})$.*

Proof. For double star $T_{\alpha,\beta}$, with $\alpha, \beta = 0$, then it is simply an edge P_2. Obviously $ID(P_2) > GA(P_2)$. If $\alpha, \beta > 0$, we have the vertex degree pairs $(\alpha+1, 1), (\beta+1, 1)$ and $(\alpha+1, \beta+1)$. So

$$ID(T_{\alpha,\beta}) - GA(T_{\alpha,\beta}) = \alpha - \frac{2\alpha\sqrt{\alpha+1}}{\alpha+2} + \beta - \frac{2\beta\sqrt{\beta+1}}{\beta+2} + \frac{\alpha+\beta+2}{(\alpha+1)(\beta+1)} - \frac{2\sqrt{(\alpha+1)(\beta+1)}}{\alpha+\beta+2} > 0,$$

which completes the proof. □

Next we need to find the class of trees which satisfies $GA(T) > ID(T)$. For this, we need the following results.

In [25], the extremal chemical trees for GA index is identified and followed by these results, in a short period of time, the first, second and third minimal (maximal) extremal chemical trees [26] are obtained. Considering the vertex version of the inverse degree and using Table 3 we have the following results.

Theorem 5.9. *Let T be a tree of order n with p pendent vertices, then*

(a) *for $n \geq 5$, the ones with only degrees one and two are the unique trees with minimum inverse degree, which is equal to $\left(\frac{n+2}{2}\right)$;*
(b) *for $n \geq 5$, the ones with a single vertex of degree three, and without vertices of degree four are the trees with second minimum inverse degree, which is equal to $\left(\frac{n+p}{2} - \frac{1}{6}\right)$;*
(c) *for $n \geq 6$, the ones with two vertices of degree three, and without vertices of degree four are the trees with the third minimum inverse degree, which is equal to $\left(\frac{n+p}{2} - \frac{1}{3}\right)$;*

Theorem 5.10. *Let T be a chemical tree of order n, then*

(i) *If $n \equiv 2 (\text{mod } 3)$, then among the $n-$vertex chemical trees,*
  (a) *for $n \geq 8$, the ones with only degrees one and four are the unique trees with the maximum inverse degree.*
  (b) *for $n \geq 8$, the ones with a unique vertex of degree two and three has the second maximum inverse degree.*
  (c) *for $n \geq 11$, the ones with exactly three vertices of degree three and without vertices of degree two has third maximum inverse degree.*

(ii) *If $n \equiv 1 (\text{mod } 3)$, then among the $n-$vertex chemical trees,*
  (a) *for $n \geq 7$, the ones with a single vertex of degree three and the remaining vertices of degree four and one, without vertices of degree two has the maximum inverse degree.*
  (b) *for $n \geq 7$, the ones with exactly two vertices of degree two, and without vertices of degree three has the second maximum inverse degree.*
  (c) *for $n \geq 10$, the ones with a single vertex of degree two and exactly two vertices of degree three has third maximum inverse degree.*

(iii) *If $n \equiv 0 (\text{mod } 3)$, then among the $n-$vertex chemical trees,*
  (a) *for $n \geq 6$, the ones with a single vertex of degree two and the remaining vertices of degree four and one, without vertices of degree three has maximum inverse degree.*

(b) *for $n \geq 9$, the ones with exactly two vertices of degree three, remaining vertices of degree four and one, and without vertices of degree two has second maximum inverse degree.*
(c) *for $n \geq 9$, the ones with a single vertex of degree three and exactly two vertices of degree two and the remaining vertices of degree four and one has third maximum inverse degree.*

Lemma 2.14, concludes that the star $K_{1,n-1}$ is the maximal tree for the inverse degree of trees. From the definition of inverse degree and Lemma 2.14, we have the following corollary

Corollary 5.11. *Let T be a tree on n vertices. Then*

(a) *for $n \geq 5$, the double star $T_{1,n-3}$ has the second maximum inverse degree.*
(b) *for $n \geq 6$, the double star $T_{2,n-4}$ has the third maximum inverse degree.*

Theorem 5.12. *Let T be a chemical tree of order $n(> 2)$ with no isolated vertices. Then $GA(T) - ID(T) > R(T) - ID(T)$.*

Proof. If T is a chemical tree, then $\Delta = 4, \delta = 1$ and for any edge $uv \in E(T)$, we have $1 < \frac{2d(u)d(v)}{d(u)+d(v)} = \frac{2\sqrt{d(u)d(v)}\sqrt{d(u)d(v)}}{d(u)+d(v)} \leq 4$. Hence, $\sum_{uv\in E(T)} \frac{1}{\sqrt{d(u)d(v)}} < \sum_{uv\in E(T)} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$. This completes the proof. □

From Theorem 5.2, we have $ID(T) - R(T) > 0$ for chemical trees, and this concludes that inverse degree and GA index are incomparable for chemical trees. So

$$\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)} - \frac{d(u)^2+d(v)^2}{d(u)^2d(v)^2} = \begin{cases} \geq -0.2451 & for\ (d(u), d(v)) = (4,1), (3,1), (2,1), \\ \geq 0.5 & for\ (d(u), d(v)) = (4,4), (4,3), (4,2), (3,3), (3,2), (2,2) \end{cases} \tag{15}$$

From Theorem 5.8, we have chemical trees isomorphic to $T_{\alpha,\beta}$ $(1 \leq \alpha, \beta \leq 4)$ with $ID(T) > GA(T)$ for $n = 2$ to 8. In addition, form (15), we get the triple star chemical trees with the property $ID(T) > GA(T)$ for the order 8 to 11, depicted in Figure 1 (right).

Spontaneously, there comes a question, is there any tree T with $GA(T) = ID(T)$? In all our attempts to find such a tree, there exits only two chemical trees T_1 and T_2 with $GA(T) = ID(T)$ depicted in Fig.2, which leads to the following conjecture.

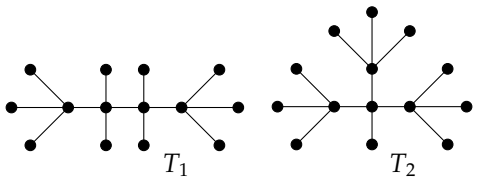

Figure 2: Chemical tress with $GA(T) = ID(T)$.

Conjecture 5.13. *If G ($\neq T_1$ or T_2) is a simple connected graph, then $ID(G) \neq GA(G)$.*

The inverse degree and GA are incomparable for the class of double and triple star chemical trees. If $n > 11$, both the double and triple star chemical trees are estimated and using Table 1, we conclude the following result.

Theorem 5.14. *Let T be a chemical tree of order $n(> 11)$ with no isolated vertices. Then $GA(T) \geq ID(T)$, with equality if and only if T is isomorphic to T_1 or T_2.*

Acknowledgement

The authors would like to give sincere gratitude the unknown reviewers for careful reading of the manuscript and for valuable comments, which greatly improved quality of our paper. The first author would like to thank his beloved Professor Kinkar Ch. Das for sending us his paper and the kind support.

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