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On the bounds of the forgotten topological index

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Abstract: The forgotten topological index is defined as the sum of cubes of the degrees of the vertices of the molecular graph G. In this paper, we obtain, analyze, and compare various lower bounds for the forgotten topological index involving the number of vertices, edges, and maximum and minimum vertex degree. Then we give Nordhaus–Gaddum-type inequalities for the forgotten topological index and coindex. Finally, we correct the number of extremal chemical trees on 15 vertices.

Key words: First Zagreb index, second Zagreb index, forgotten topological index

1. Introduction

Throughout this paper, we consider G to be a simple connected graph with $|V(G)| = n$ vertices and $|E(G)| = m$ edges. The degree of a vertex $v_i (1 \leq i \leq n)$ is denoted by $d(v_i)$ such that $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$. In particular, Δ, Δ_2, and δ are called the first, second maximum, and minimum degrees of G, respectively. Let $\overline{G}$ denote the complement graph of G with the same vertex set $V(G)$ in which two vertices u and v are adjacent if and only if they are not adjacent in G. The line graph $L(G)$ is obtained from G in which $V(L(G)) = E(G)$, where two vertices of $L(G)$ are adjacent if and only if they are adjacent edges of G.

In 1972, Gutman and Trinajstić introduced the classical Zagreb indices in [13] and they are among the oldest and most used molecular structure-descriptors. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined as

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

There is much research regarding the mathematical and chemical properties for Zagreb indices available in the literature and we refer the reader to [5, 8] for the recent results and for more information on the Zagreb indices.

In 1987, Naurmi [18] introduced the inverse degree and it attracted attention through conjectures of the computer program Graffiti [10]. The inverse degree of a graph G with no isolated vertices is defined as

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

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The harmonic index $H(G)$ also first emerged in the conjectures of the computer program Graffiti [10], defined by

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

In 1997, Albertson [2] introduced the imbalance of an edge $e = uv \in E(G)$ as $|d(u) - d(v)|$ and the irregularity of G as

$$irr(G) = \sum_{uv \in E(G)} |d(u) - d(v)|.$$

In 2005, Li and Zheng [15] introduced the first general Zagreb index. Subsequently, two of the present authors together with Gutman [5] introduced the second general Zagreb index and these indices are defined as

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

It is easily seen that for any graph G, we have

$$M_1^{\alpha+1}(G) = \sum_{v \in V(G)} d(v)^{\alpha+1} = \sum_{uv \in E(G)} [d(u)^\alpha + d(v)^\alpha]. \tag{1.1}$$

In recent years, some novel variants of ordinary Zagreb indices have been introduced and studied. In particular, the first and second Zagreb coindices are defined [4] as

$$\overline{M}_1 = \overline{M}_1(G) = \sum_{uv \notin E(G)} [d(u)+d(v)] \quad \text{and} \quad \overline{M}_2 = \overline{M}_2(G) = \sum_{uv \notin E(G)} d(u)d(v).$$

The first and second Zagreb indices are successfully used in the investigation of the structure-dependency of the total π-electron energy (ε). It was found that (ε) depends on $M_1(G)$ and thus provides a measure of the carbon skeleton of the underlying molecules. In the same paper, another topological index, defined as the sum of cubes of degrees of the vertices of the graph, was also shown to influence (ε).

In 2015, Furtula and Gutman [11] reinvestigated this index; they showed that the predictive ability of this index is similar to that of the first Zagreb index and that for the entropy and acentric factor, both of them yield correlation coefficients greater than 0.95. They named this index the *forgotten topological index* or *F-index*, denoted by $F(G)$. Some bounds for the forgotten topological index are seen in [11] and the extremal values of the *F-index* for trees are seen in [1]. Note that for $\alpha = 1, 2$ in (1.1) they are simply the first Zagreb index $M_1^2(G)$ and forgotten topological index $M_1^3(G)$, respectively.

This paper is organized as follows. In Section 3, we present some new lower bounds on the forgotten topological index $F(G)$ and forgotten topological coindex $\overline{F}(G)$ of graph G in terms of $n, m, \Delta, \Delta_2, \delta$, and $M_1(G)$. We also give lower bounds on $F(G) + F(\overline{G})$ and $\overline{F}(G) + \overline{F}(\overline{G})$.

2. Preliminaries

Let P_n, $K_{1,n-1}$, C_n, and W_n denote the *path, star, cycle, and wheel* graphs on n vertices, respectively. The *helm* H_n is obtained from the wheel graph W_{n-1} by adjoining a pendant edge at each vertex of the cycle. The *crown* Cr_n is obtained from the helm graph H_n by deleting the maximum degree vertex of the helm. The *flower* Fl_n is obtained from the helm H_n by joining each pendent vertex to the central vertex of the helm. The *web* $W(2,n)$ is obtained from H_n by joining the pendent vertices to form a cycle C_{n-1} and then adding a pendent edge to each vertex of its outer cycle.

The *vertex-semitotal graph* $T_1(G)$ is a graph with vertex set $V(G) \cup V(E)$, such that any two vertices $u, v \in V(T_1(G))$ are adjacent if and only if (i) $uv \in E(G)$; (ii) one is a vertex of G and the other is an edge of G incident on it. The *edge-semitotal graph* $T_2(G)$ is a graph with vertex set $V(G) \cup V(E)$, such that any two vertices $u, v \in V(T_2(G))$ are adjacent if and only if (i) u and v are adjacent edges in G; (ii) one is a vertex of G and the other is an edge of G incident on it.

A graph G is called *bidegreed* if its vertex degree is either Δ or δ with $\Delta > \delta \geq 1$. Let Γ be the class of graphs such that $d(v_i) = \delta$, $2 \leq i \leq n$. Note that Γ is a special case of the bidegreed graphs. Let Ω be the class of graphs such that $d(v_1) \geq d(v_2) > d(v_i)$ with $d(v_i) = \delta, i = 3, 4, \ldots, n$. Let Θ be the class of graphs such that $d(v_1) > d(v_i)$ with $d(v_2) = \cdots = d(v_{n-1}) = \Delta_2, d(v_n) = \delta, i = 2, 3, \ldots, n$, respectively. If $\Delta_2 = \delta$, then Γ and Θ are in the same class. The edge imbalance of an edge is the absolute value of the difference of its two end vertex degrees. A *biregular* graph is a special type of bidegreed bipartite graph, which has constant edge imbalance.

In 1998, de Caen [9] obtained the lower bound for the first Zagreb index in the context of the sum of squares of degrees of a graph.

Lemma 2.1 [9] *Let G be a graph with n vertices and m edges. Then*

$$M_1(G) \geq \frac{4m^2}{n} \tag{2.1}$$

with equality if and only if G is regular.

In 2006, Ciobă [7] obtained the lower bound for the first general Zagreb index.

Lemma 2.2 [7] *If G is a connected graph and α is a positive number, then*

$$M_1^{\alpha+1}(G) \geq \left(\frac{2m}{n}\right) M_1^{\alpha}(G) \tag{2.2}$$

with equality if and only if G is regular.

Later, in 2012, Ilić and Zhou [14] obtained the lower bound for $F(G)$, which is a special case formula for (2.2) at $\alpha = 2$. In 2009, Zhou and Trinajstić [21] obtained the following lower bound in the context of the general sum-connectivity index.

Lemma 2.3 [21] *Let G be a graph with n vertices and m edges. Then*

$$F(G) \geq \frac{16m^3}{n^2} - 2M_2(G) \tag{2.3}$$

with equality if and only if G is regular.

Lemma 2.4 [21] *Let G be a graph with $m \geq 1$ edges. If $0 < \alpha < 1$, then $\chi^{\alpha}(G) \leq M_1(G)^{\alpha} m^{1-\alpha}$, and if $\alpha < 0$ or $\alpha > 1$, then $\chi^{\alpha}(G) \geq M_1(G)^{\alpha} m^{1-\alpha}$, and either equality holds if and only if $d(u)+d(v)$ is a constant for any edge uv.*

Very recently, Furtula et al. [11, 12] presented the following lower bounds for the F-index.

Lemma 2.5 [11] *Let G be a graph with n vertices and m edges. Then*

$$F(G) \geq \frac{(M_1(G))^2}{2m} \tag{2.4}$$

with equality if and only if G is regular.

Lemma 2.6 [11] *Let G be a graph with n vertices and m edges. Then*

$$F(G) \geq \frac{(M_1(G))^2}{m} - 2M_2(G) \tag{2.5}$$

with equality if and only if G is regular.

Lemma 2.7 [12] *Let G be a graph with n vertices and m edges. Then*

$$F(G) \geq \frac{2m}{n} M_1(G) \tag{2.6}$$

with equality if and only if G is regular.

Remark 2.8 *Note that, for $\alpha = 2$ in Lemma 2.2 and Lemma 2.4, it has (2.6) and (2.5) as its special cases, respectively. Also from Lemma 2.4, it is clear that the equality of (2.5) holds if and only if $d(u)+d(v)$ is a constant for any edge uv. A typo in inequality (2.4) in [12] leads to the conclusion that (2.6) is an improvement for (2.4). Using inequality (2.1), we conclude that the lower bound (2.4) is always better than (2.6); that is,*

$$F(G) \geq \frac{(M_1(G))^2}{2m} \geq \frac{M_1(G)}{2m} \cdot \frac{4m^2}{n} = \left(\frac{2m}{n}\right) M_1(G).$$

Furthermore, the lower bound (2.5) is always better than (2.3):

$$F(G) \geq \frac{(M_1(G))^2}{m} - 2M_2(G) \geq \frac{1}{m} \cdot \left(\frac{4m^2}{n}\right)^2 - 2M_2(G) = \frac{16m^3}{n^2} - 2M_2(G).$$

3. Main results

At first, we prove the following theorems that establish the new lower bounds for $F(G)$ in terms of $n, m, \Delta, \Delta_2, \delta, ID(G)$, and $M_1(G)$.

Theorem 3.1 *Let G be a simple graph of order $n(\geq 3)$ with no isolated vertices. Then*

$$F(G) \geq \Delta^3 + \Delta_2^3 + \Phi_1^* \tag{3.1}$$

with equality if and only if G is regular or $G \in \Gamma$ or $G \in \Omega$, where

$$\Phi_1^* = \frac{\left[M_1(G) - \Delta^2 - \Delta_2^2\right]^2 + (2m - \Delta - \Delta_2)\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\Delta_2}\right) - (n-2)^2}{(2m - \Delta - \Delta_2)}.$$

Proof Consider $w_1, w_2, \ldots, w_r$ to be the nonnegative weights; then we have the weighted version of the Cauchy–Schwartz inequality:

$$\sum_{i=1}^{r} w_i a_i^2 \sum_{i=1}^{r} w_i b_i^2 \geq \left(\sum_{i=1}^{r} w_i a_i b_i \right)^2. \tag{3.2}$$

Since w_i is nonnegative, we assume that $w_i = x_i - y_i$ such that $x_i \geq y_i \geq 0$. Thus,

$$\sum_{i=1}^{r} x_i a_i^2 \sum_{i=1}^{r} x_i b_i^2 - \left(\sum_{i=1}^{r} x_i a_i b_i \right)^2 \geq \sum_{i=1}^{r} y_i a_i^2 \sum_{i=1}^{r} y_i b_i^2 - \left(\sum_{i=1}^{r} y_i a_i b_i \right)^2 \geq 0. \tag{3.3}$$

By our assumption, G has no isolated vertices and so we have $\frac{1}{d(v_i)} \leq 1$, for all $v_i \in V(G)$. Thus, by fixing $r = n-2$, $x_i = d(v_{i+2})$, $y_i = \frac{1}{d(v_{i+2})}$, $a_i = d(v_{i+2})$, and $b_i = 1$, for all $i = 1, 2, \ldots, r$ in the above, we get

$$\sum_{i=3}^{n} d(v_i)^3 \sum_{i=3}^{n} d(v_i) - \left(\sum_{i=3}^{n} d(v_i)^2 \right)^2 \geq \sum_{i=3}^{n} d(v_i) \sum_{i=3}^{n} \frac{1}{d(v_i)} - \left(\sum_{i=3}^{n} 1 \right)^2.$$

Using

$$\sum_{i=3}^{n} d(v_i)^3 = F(G) - \Delta^3 - \Delta_2^3, \quad \sum_{i=3}^{n} d(v_i)^2 = M_1(G) - \Delta^2 - \Delta_2^2, \tag{3.4}$$

$$\sum_{i=3}^{n} d(v_i) = 2m - \Delta - \Delta_2 \quad \text{and} \quad \sum_{i=3}^{n} \frac{1}{d(v_i)} = ID(G) - \frac{1}{\Delta} - \frac{1}{\Delta_2} \tag{3.5}$$

completes the proof. □

If we set $r = n-2$, $x_i = d(v_{i+1})$, $y_i = \frac{1}{d(v_{i+1})}$, $a_i = d(v_{i+1})$, and $b_i = 1$ in (3.3) for all $i = 1, 2, \ldots, r$, we have the following result.

Corollary 3.2 *With the assumptions in Theorem 3.5, one has the inequality*

$$F(G) \geq \Delta^3 + \delta^3 + \Phi_2^* \tag{3.6}$$

with equality if and only if G is regular or $G \in \Gamma$ or $G \in \Theta$, where

$$\Phi_2^* = \frac{\left[M_1(G) - \Delta^2 - \delta^2\right]^2 + (2m - \Delta - \delta)\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\delta}\right) - (n-2)^2}{(2m - \Delta - \delta)}.$$

Remark 3.3 *In [11], it is shown that (2.4) and (2.5) are incomparable. It is interesting to see that both the lower bounds (2.5) and (2.4) coincide together for the web $W(t,7)$ and $W(t,7) - v_n$, other than the equality case.*

By setting $x_i = d(v_i)$, $y_i = 0$, $a_i = d(v_i)$, and $b_i = 1$ in (3.3) immediately has (2.4) as its special case. Also, by comparing the choice of selection of y_i in both the cases, it is easy to see that the lower bounds (3.1) and (3.6) are always better than (2.4). Refer to Figure 1 for the lower bound comparison of all 18 isomers of octane.

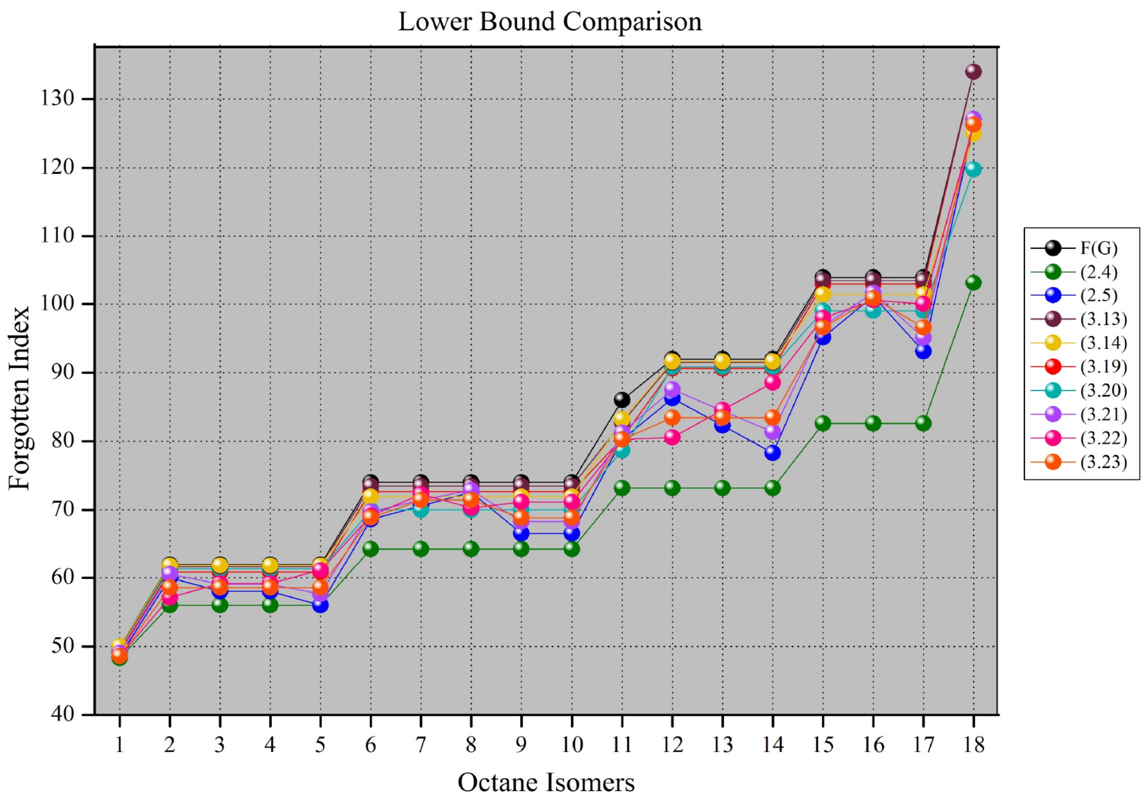

Figure 1. Lower bound comparison for $F(G)$ for 18 isomers of octane.

Remark 3.4 *The lower bounds* (3.1) *and* (3.6) *are incomparable. Namely, there exists a molecular graph of 1,2-diethylcyclopentane for which* (3.1) *is better than* (3.6) *and there exists a molecular graph of 1,1-diethylcyclopentane for which* (3.6) *is better than* (3.1).

Next, we refine our own lower bounds (3.1) and (3.6) and give the new successors for these lower bounds.

Theorem 3.5 *Let G be a simple graph of order $n(\geq 3)$. Then*

$$F(G) \geq \Delta^3 + \Delta_2^3 + \Phi_3^* \tag{3.7}$$

with equality if and only if G is regular or $G \in \Gamma$ or $G \in \Omega$, where

$$\Phi_3^* = \frac{\left[M_1(G) - \Delta^2 - \Delta_2^2\right]^2 + (n-2)\left[M_1(G) - \Delta^2 - \Delta_2^2\right]}{(2m - \Delta - \Delta_2)} - (2m - \Delta - \Delta_2).$$

Proof Using the inequality (3.3) and by fixing $r = n-2$, $x_i = d(v_{i+2})$, $y_i = 1$, $a_i = d(v_{i+2})$, and $b_i = 1$, for all $i = 1, 2, \ldots, r$, we get

$$\sum_{i=3}^{n} d(v_i)^3 \sum_{i=3}^{n} d(v_i) - \left(\sum_{i=3}^{n} d(v_i)^2\right)^2 \geq (n-2)\sum_{i=3}^{n} d(v_i)^2 - \left(\sum_{i=3}^{n} d(v_i)\right)^2,$$

where we used (3.4) and (3.5) to complete the proof. □

Next, by setting $r=n-2$, $a_i=d(v_{i+1})$, $x_i=d(v_{i+1})$, $b_i=1$, and $y_i=1$ in (3.3) for all $i=1,2,\ldots,r$, we have the following corollary.

Corollary 3.6 *With the assumptions in Theorem 3.1, one has the inequality*

$$F(G)\geq \Delta^3+\delta^3+\Phi_4^* \tag{3.8}$$

with equality if and only if G is regular or $G\in\Gamma$ or $G\in\Theta$, where

$$\Phi_4^*=\frac{\left(M_1(G)-\Delta^2-\delta^2\right)^2+(n-2)\left(M_1(G)-\Delta^2-\delta^2\right)}{(2m-\Delta-\delta)}-(2m-\Delta-\delta).$$

Remark 3.7 *For each graph G, our aim is to show that (3.7) and (3.8) are always better than the lower bounds in (3.1) and (3.6) respectively. For this, we have to claim that*

$$\Phi_3^*\geq\Phi_1^*,\ \Phi_4^*\geq\Phi_2^*.$$

Recalling inequality (3.3) and by fixing $r=n-2$, $x_i=1, y_i=\frac{1}{d(v_{i+2})}, a_i=d(v_{i+2})$, and $b_i=1$ with $i=1,2,\ldots,r$, we have

$$\begin{aligned}&\left(M_1(G)-\Delta^2-\Delta_2^2\right)(n-2)-(2m-\Delta-\Delta_2)^2\\ &\qquad\qquad\geq(2m-\Delta-\Delta_2)\left(ID(G)-\frac{1}{\Delta}-\frac{1}{\Delta_2}\right)-(n-2)^2.\end{aligned}$$

Adding $\left(M_1(G)-\Delta^2-\Delta_2^2\right)^2$ and dividing by $(2m-\Delta-\Delta_2)$ on both sides of the above inequality completes our claim of $\Phi_3^*\geq\Phi_1^*$. In an analogous manner we complete our second claim.

Intuitively one may conjecture that $\Phi_4^*\underset{?}{\geq}\Phi_1^*$ and $\Phi_3^*\underset{?}{\geq}\Phi_2^*$. However, it is not true, as for the molecular graph 1,2-diethylcyclobutane (3.1) is better than (3.8) and for 1,1-diethylcyclobutane (3.6) is better than (3.7).

We are still not satisfied with our previous lower bounds. Next, we are ready to improve our own bounds for the forgotten topological index.

Theorem 3.8 *Let G be a simple graph of order $n(\geq 3)$ with no isolated vertices. Then*

$$F(G)\geq\Delta^3+\Delta_2^3+\Upsilon_1^* \tag{3.9}$$

with equality if and only if G is regular or $G\in\Gamma$ or $G\in\Omega$, where

$$\Upsilon_1^*=\frac{\left[\left(M_1(G)-\Delta^2-\Delta_2^2\right)+\sqrt{(2m-\Delta-\Delta_2)\left(ID(G)-\frac{1}{\Delta}-\frac{1}{\Delta_2}\right)-(n-2)}\right]^2}{(2m-\Delta-\Delta_2)}.$$

Proof Consider $w_1,w_2,\ldots,w_r$ to be the nonnegative weights; then, from (3.2), we have

$$\left(\sum_{i=1}^{r}w_ia_i^2\right)^{\frac{1}{2}}\left(\sum_{i=1}^{r}w_ib_i^2\right)^{\frac{1}{2}}\geq\sum_{i=1}^{r}w_ia_ib_i. \tag{3.10}$$

Since w_i is nonnegative, we assume that $w_i = x_i - y_i$ such that $x_i \geq y_i \geq 0$. Thus,

$$\left(\sum_{i=1}^{r} x_i a_i^2\right)^{\frac{1}{2}} \left(\sum_{i=1}^{r} x_i b_i^2\right)^{\frac{1}{2}} - \sum_{i=1}^{r} x_i a_i b_i \geq \left(\sum_{i=1}^{r} y_i a_i^2\right)^{\frac{1}{2}} \left(\sum_{i=1}^{r} y_i b_i^2\right)^{\frac{1}{2}} - \sum_{i=1}^{r} y_i a_i b_i \geq 0. \tag{3.11}$$

By setting $r = n-2$, $a_i = d(v_{i+2})$ and $b_i = 1$, for all $i = 1, 2, \ldots, r$ and by fixing $x_i = d(v_{i+2})$ and $y_i = \frac{1}{d(v_{i+2})}$ in the above, we complete the proof. □

Corollary 3.9 *With the assumptions in Theorem 3.8, one has the inequality*

$$F(G) \geq \Delta^3 + \delta^3 + \Upsilon_2^* \tag{3.12}$$

with equality if and only if G is regular or $G \in \Gamma$ or $G \in \Theta$, where

$$\Upsilon_2^* = \frac{\left[\left(M_1(G) - \Delta^2 - \delta^2\right) + \sqrt{(2m - \Delta - \delta)\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\delta}\right)} - (n-2)\right]^2}{(2m - \Delta - \delta)}.$$

First we have to prove that (3.9) is always better than (3.1). For this we have to prove $\Upsilon_1^* \geq \Phi_1^*$. Considering inequality (3.2) and providing $w_i = d(v_{i+2})$, $a_i = \frac{1}{d(v_{i+2})}$, and $b_i = 1$, we get $\sqrt{(2m - \Delta - \Delta_2)(ID(G) - 1/\Delta - 1/\Delta_2)} \geq (n-2)$. It is easy to see that $(M_1(G) - \Delta^2 - \Delta_2^2) - (n-2) \geq 0$. Thus, by multiplying it on both sides of the above inequality, we get

$$2\left(M_1(G) - \Delta^2 - \Delta_2^2\right)\sqrt{(2m - \Delta - \Delta_2)\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\Delta_2}\right)} + 2(n-2)^2$$

$$\geq 2(n-2)\sqrt{(2m - \Delta - \Delta_2)\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\Delta_2}\right)} + 2(n-2)\left(M_1(G) - \Delta^2 - \Delta_2^2\right).$$

Adding $\left(M_1(G) - \Delta^2 - \Delta_2^2\right)^2 + (2m - \Delta - \Delta_2)(ID(G) - 1/\Delta - 1/\Delta_2)$ and dividing by $(2m - \Delta - \Delta_2)$ on both sides of the above inequality leads to the conclusion $\Upsilon_1^* \geq \Phi_1^*$. Analogously, we can prove that $\Upsilon_2^* \geq \Phi_2^*$, but, on the other hand, Υ_1^* and Υ_2^* are incomparable.

Remark 3.10 *The lower bounds (3.9) and (3.12) are matchless. For the graphs Fl_n and $L(Fl_n)$, (3.12) is finer than (3.9) and for $T_2(Fl_n)$ and $T_1[L(Fl_n)]$, (3.9) is finer than (3.12) (Table 1):*

Table 1. Lower bounds.

	Fl_{15}	$T_2(Fl_{15})$	$L(Fl_{15})$	$T_1[L(Fl_{15})]$
n	31	91	60	600
m	60	660	540	1620
$F(G)$	28080	1120080	900720	7210080
(3.9)	28013.501	955958.802	816347.027	4616746.829
(3.12)	28015.492	955287.95	817804.321	4571543.636

Theorem 3.11 *Let G be a simple graph of order $n(\geq 3)$. Then*

$$F(G) \geq \Delta^3 + \Delta_2^3 + \Upsilon_3^* \tag{3.13}$$

with equality if and only if G is regular or $G \in \Gamma$ or $G \in \Omega$, where

$$\Upsilon_3^* = \frac{\left[\left(M_1(G) - \Delta^2 - \Delta_2^2\right) + \sqrt{(n-2)\left(M_1(G) - \Delta^2 - \Delta_2^2\right)} - (2m - \Delta - \Delta_2)\right]^2}{(2m - \Delta - \Delta_2)}.$$

Proof The proof follows by the same terminology of Theorem 3.8 by fixing $r = n-2$, $x_i = d(v_{i+2})$, $y_i = 1$, $a_i = d(v_{i+2})$, and $b_i = 1$, for all $i = 1, 2, \cdots, r$. □

Corollary 3.12 *Let G be a simple graph of order $n(\geq 3)$. Then*

$$F(G) \geq \Delta^3 + \delta^3 + \Upsilon_4^* \tag{3.14}$$

with equality if and only if G is regular or $G \in \Gamma$ or $G \in \Theta$, where

$$\Upsilon_4^* = \frac{\left[\left(M_1(G) - \Delta^2 - \delta^2\right) + \sqrt{(n-2)\left(M_1(G) - \Delta^2 - \delta^2\right)} - (2m - \Delta - \delta)\right]^2}{(2m - \Delta - \delta)}.$$

Next, we have to prove that the lower bound (3.13) is always better than (3.7), i.e. we have to show that $\Upsilon_3^* \geq \Phi_3^*$. Starting with inequality (3.2) and replacing $r = n-2, a_i = d(v_{i+2}), b_i = 1$, and $w_i = 1$, we get

$$\sqrt{(n-2)\left(M_1(G) - \Delta^2 - \Delta_2^2\right)} - (2m - \Delta - \Delta_2) \geq 0. \tag{3.15}$$

It is easy to see that

$$\left(M_1(G) - \Delta^2 - \Delta_2^2\right) \geq (2m - \Delta - \Delta_2). \tag{3.16}$$

By multiplying (3.15) and (3.16), then by adding the terms $(n-2)\left(M_1(G) - \Delta^2 - \Delta_2^2\right)$ and $\left(M_1(G) - \Delta^2 - \Delta_2^2\right)^2$, and then by dividing both sides by $(2m - \Delta - \Delta_2)$, we get $\Upsilon_3^* \geq \Phi_3^*$. In the same way, we have that $\Upsilon_4^* \geq \Phi_4^*$.

In analogy to Remark 3.7, one can prove that $\Upsilon_3^* \geq \Upsilon_1^*$ and $\Upsilon_4^* \geq \Upsilon_2^*$ and we leave the proof for the interested reader.

Remark 3.13 *From the above arguments, we conclude that $\Upsilon_3^* \geq \Upsilon_1^* \geq \Phi_1^*$ and $\Upsilon_4^* \geq \Upsilon_2^* \geq \Phi_2^*$. However, in the same way, one can conjecture that $\Upsilon_1^* \underset{?}{\geq} \Phi_3^*$. It is not true in general; see the following example for the comparison of the lower bounds (3.9) and (3.7) (Table 2):*

Let G and H be any graph. Then $\sigma_G(H)$ denotes the number of distinct subgraphs of the graph G that are isomorphic to H. In 2014, one of the present authors with Gutman [5] established the counting relation for $F(G)$ in terms of counting the total number of stars in a given graph.

Table 2. Comparison of the lower bounds (3.9) and (3.7).

	H_6	$L(H_6)$	$\overline{L(H_6)}$
n	13	18	18
m	18	51	102
$F(G)$	606.0	4530.0	28824.0
(3.9)	582.805	4257.69	28129.816
(3.7)	574.846	4253.023	28129.909

Proposition 3.14 [5] *Let G be a simple graph. Then*

$$F(G) = 6\sigma_G(K_{1,3}) + 6\sigma_G(K_{1,2}) + 2m, \tag{3.17}$$

$$F(G) = 6\sigma_G(K_{1,3}) + 3M_1(G) - 4m. \tag{3.18}$$

In addition, we now give an identity for the forgotten topological index in terms of the general sum connectivity index and some class subgraph counting in G.

Proposition 3.15 *Let G be a simple graph. Then*

$$F(G) = \chi^2(G) - 2\sigma_G(P_4) - 4\sigma_G(P_3) - 6\sigma_G(C_3) - 2m.$$

Proof Using the definition of the general sum connectivity index and the identity for the second Zagreb index [5], we have that $M_2(G) = \sigma_G(P_4) + 2\sigma_G(P_3) + 3\sigma(C_3) + m$, which completes the proof. □

From [16], we have $M_1(G) \geq \Delta^2 + \Delta_2^2 + \Psi_1^*$, $M_1(G) \geq \Delta^2 + \delta^2 + \Psi_2^*$, and using (3.18), we give some new and strong lower bounds for the forgotten topological index.

Theorem 3.16 *Let G be a simple graph of order $n(\geq 3)$ with no isolated vertices. Then*

$$F(G) \geq 3\Delta^2 + 3\Delta_2^2 + 3\Psi_1^* + 6\sigma_G(K_{1,3}) - 4m \tag{3.19}$$

with equality if and only if G is regular or $G \in \Gamma$ or $G \in \Omega$, where

$$\Psi_1^* = \frac{\left((2(m+1) - n - \Delta - \Delta_2) + \sqrt{(2m - \Delta - \Delta_2)\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\Delta_2}\right)}\right)^2}{n-2}.$$

Corollary 3.17 *Let G be a simple graph of order $n(\geq 3)$ with no isolated vertices. Then*

$$F(G) \geq 3\Delta^2 + 3\delta^2 + 3\Psi_2^* + 6\sigma_G(K_{1,3}) - 4m \tag{3.20}$$

with equality if and only if G is regular or $G \in \Gamma$ or $G \in \Theta$, where

$$\Psi_2^* = \frac{\left((2(m+1) - n - \Delta - \delta) + \sqrt{(2m - \Delta - \delta)\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\delta}\right)}\right)^2}{n-2}.$$

Remark 3.18 *In [16], the present authors proved that Ψ_1^* and Ψ_2^* are incomparable. In addition, the lower bounds (3.19), (3.13), (3.20), and (3.14) are also incomparable respectively (Table 3):*

Table 3. Comparison of the lower bounds (3.19), (3.13), (3.20), and (3.14).

	n	m	$F(G)$	(3.19)	(3.20)	(3.13)	(3.14)
$W(2,15)$	46	75	5310	5228.3	5235.443	5295.659	5297.542
$T_1(W(2,15))$	121	225	43080	41192.289	41155.235	40548.176	40541.287
$T_2(W(2,15))$	121	435	133110	126445.071	126136.04	107890.171	106750.598

Next, we improve inequality (2.5) for the forgotten index $F(G)$ using the harmonic index $H(G)$.

Theorem 3.19 *Let G be a simple connected graph of order $n(\geq 3)$. Then*

$$F(G) \geq \frac{M_1(G)}{m}\left(2H(G) + M_1(G)\right) - 2M_2(G) - 4m, \tag{3.21}$$

where equality holds if and only if $d(u)+d(v)$ is constant for any edge uv.

Proof By our assumption $n \geq 3$, for any edge $uv \in E(G)$, $d(u)+d(v) > 2$ and using inequality (3.3), by fixing $r = m$, $x_i = d(u)+d(v)$, $y_i = 2$, $a_i = \sqrt{d(u)+d(v)}$, and $b_i = \frac{1}{\sqrt{d(u)+d(v)}}$, we get

$$\sum_{uv\in E(G)} (d(u)+d(v))^2 \sum_{uv\in E(G)} 1 - \left(\sum_{uv\in E(G)} (d(u)+d(v))\right)^2$$

$$\geq \sum_{uv\in E(G)} 2\,(d(u)+d(v)) \sum_{uv\in E(G)} \frac{2}{d(u)+d(v)} - \left(2\sum_{uv\in E(G)} 1\right)^2$$

$$\left(F(G) + 2M_2(G)\right)m - \left(M_1(G)\right)^2 \geq 2M_1(G)H(G) - 4m^2,$$

which completes the proof. □

Remark 3.20 *Using the Cauchy–Schwartz inequality, it is easy to see that $M_1(G)H(G) - 2m^2 \geq 0$, which concludes that the lower bound in (3.21) is always better than (2.5).*

Very recently, Che and Chen [6] presented the following lower bounds in terms of irregularity of the graph G.

Lemma 3.21 [6] *Let G be a connected graph with m edges*

$$F(G) \geq \frac{irr^2(G)}{m} + 2M_2(G), \tag{3.22}$$

where equality holds if and only if $|d(u)-d(v)|$ is constant for all edges uv of G.

Lemma 3.22 [6] *Let G be a connected graph with m edges*

$$F(G) \geq \frac{irr^2(G) + M_1(G)^2}{2m}, \tag{3.23}$$

where equality holds if and only if G is regular or biregular.

Remark 3.23 *It is interesting to see that our lower bounds are incomparable with the bounds given in Lemma 3.21 and Lemma 3.22 (Table 4):*

Table 4. Our lower bounds, Lemma 3.21, and Lemma 3.22.

	$F(G)$	(3.19)	(3.20)	(3.13)	(3.14)	(3.21)	(3.22)	(3.23)
Cr_6	168	155.948	157.282	163.984	165.082	158	156	156
$L(Cr_6)$	432	413.096	413.029	415.135	416.240	417.333	416	416
$T_1(Cr_6)$	1440	1317.589	1297.954	1275.261	1262.972	1264	1312	1280
$T_2(Cr_6)$	1848	1757.666	1755.619	1760.189	1752.480	1675.205	1800	1731.429

One of the present authors with Song gave the relation for the first general Zagreb index and its coindex [17].

Theorem 3.24 *Let G be a simple graph on n vertices and m edges. For $\alpha \geq 1$,*

$$\overline{M}_1^{\alpha+1}(G) = (n-1)M_1^{\alpha}(G) - M_1^{\alpha+1}(G).$$

Based on Theorems 3.11, 3.12, and 3.24, the following bounds for the forgotten topological coindex hold immediately.

Corollary 3.25 *Let G be a simple graph with n vertices, m edges, maximum degree Δ, second maximum degree Δ_2, and minimum degree δ. Then*

$$\overline{F}(G) \leq (n-1)M_1(G) - \left[\Delta^3 + \Delta_2^3 + \Upsilon_3^*\right]$$

with equality if and only if G is regular or $G \in \Gamma$ or $G \in \Omega$, and

$$\overline{F}(G) \leq (n-1)M_1(G) - \left[\Delta^3 + \delta^3 + \Upsilon_4^*\right]$$

with equality if and only if G is regular or $G \in \Gamma$ or $G \in \Theta$.

Corollary 3.26 *Let G be a simple graph with n nonisolated vertices, m edges, maximum degree Δ, second maximum degree Δ_2, and minimum degree δ. Then*

$$\overline{F}(G) \geq (n-1)\left[\Delta^2 + \Delta_2^2 + \Psi_1^*\right] - F(G)$$

with equality if and only if G is regular or $G \in \Gamma$ or $G \in \Omega$, and

$$\overline{F}(G) \geq (n-1)\left[\Delta^2 + \delta^2 + \Psi_2^*\right] - F(G)$$

with equality if and only if G is regular or $G \in \Gamma$ or $G \in \Theta$.

In [20], the following Nordhaus–Gaddum-type inequality for $F(G) + F(\overline{G})$ was established in terms of vertices:

$$F(G) + F(\overline{G}) \geq \frac{n(n-1)^3}{4}. \tag{3.24}$$

Now we give new lower bounds on $F(G) + F(\overline{G})$ in terms of n, m, Δ, δ, and $ID(G)$.

Theorem 3.27 *Let G be a simple graph with n nonisolated vertices, m edges, maximum degree Δ, second maximum degree Δ_2, and minimum degree δ. Then*

$$F(G)+F\left(\overline{G}\right)\geq n(n-1)^3-6m(n-1)^2+3(n-1)\left[\Delta^2+\Delta_2^2+\Psi_1^*\right]$$

with equality if and only if G is regular or $G\in\Gamma$ or $G\in\Omega$, and

$$F(G)+F\left(\overline{G}\right)\geq n(n-1)^3-6m(n-1)^2+3(n-1)\left[\Delta^2+\delta^2+\Psi_2^*\right]$$

with equality if and only if G is regular or $G\in\Gamma$ or $G\in\Theta$.

Proof It is easy to see that

$$\begin{aligned}F\left(\overline{G}\right)&=\sum_{i=1}^{n}\left(n-1-d_G\left(v_i\right)\right)^3\\&=n(n-1)^3-6m(n-1)^2+3(n-1)M_1(G)-F(G).\end{aligned}$$

Using the inequalities $M_1(G)\geq\Delta^2+\Delta_2^2+\Psi_1^*, M_1(G)\geq\Delta^2+\delta^2+\Psi_2^*$ from [16] in the above completes our claim. □

On the other hand, Nordhaus–Gaddum-type inequalities for the first Zagreb coindex were established in terms of vertices in [19]. In analogy, we now establish the lower bounds for $\overline{F}(G)+\overline{F}\left(\overline{G}\right)$.

Corollary 3.28 *Let G be a simple graph with n nonisolated vertices, m edges, maximum degree Δ, second maximum degree Δ_2, and minimum degree δ. Then*

$$\begin{aligned}\overline{F}(G)+\overline{F}\left(\overline{G}\right)\geq{}& n(n-1)^3-4m(n-1)^2-\left[F(G)+F\left(\overline{G}\right)\right]\\&+2(n-1)\left(\Delta^2+\Delta_2^2+\Psi_1^*\right)\end{aligned}$$

with equality if and only if G is regular or $G\in\Gamma$ or $G\in\Omega$, and

$$\begin{aligned}\overline{F}(G)+\overline{F}\left(\overline{G}\right)\geq{}& n(n-1)^3-4m(n-1)^2-\left[F(G)+F\left(\overline{G}\right)\right]\\&+2(n-1)\left(\Delta^2+\delta^2+\Psi_2^*\right)\end{aligned}$$

with equality if and only if G is regular or $G\in\Gamma$ or $G\in\Theta$.

Proof For $\alpha=2$ in Theorem 3.24, we have $\overline{F}(G)=(n-1)M_1(G)-F(G)$. Rewriting Theorem 3.24 for the complement graph of G, one can see the following result about co-complement, $\overline{F}(\overline{G})=(n-1)M_1(\overline{G})-F(\overline{G})$. Using the above results with Theorem 2.25 of [16] completes our claim. □

4. Computational results

For computational purposes, we use the software GraphTea (see [3]) considering various phases of testing. GraphTea is graph visualization software designed specifically to visualize and explore graph algorithms and the topological indices interactively. In [1], all the extremal chemical trees were obtained up to 20 vertices, in which the degree sequence as well as all corresponding trees were obtained by an exhaustive computer search using the mathematical software Sage for n = 20 that took several hours. GraphTea is a better tool, specially

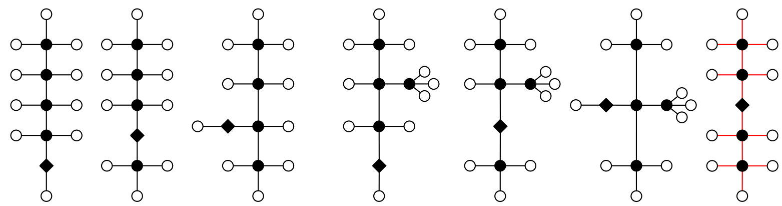

Figure 2. Extremal chemical trees for $F(G)$ with 15 vertices.

designed to extract both the adjacency matrix and the corresponding graph with their specified topological indices in a shorter time interval. In the search for the extremal chemical trees for $F(G)$, an extremal chemical tree for $n = 15$ was missed in [1], as demonstrated in Figure 2.

Table 5 provides the computational results for the connected graphs on $n = 3$ to 9 vertices and trees on $n = 10$ to 20 vertices. In the 'Parameter' section of Tables 5 and 6, the first three columns represent the degree of the vertex n, total number of connected graphs (trees) on n vertices, and average value of the forgotten topological index $F(G)$. The next six sections of three columns represent the average value of the lower bounds, the standard deviation

$$\left(\sqrt{\frac{\sum_G (F(G) - X(G))^2}{count}}\right),$$

and the number of graphs holding equality.

Table 5. Lower bound comparison of $F(G)$ for simple connected graphs up to 9 vertices.

Parameters			Theorem 3.11			Corollary 3.12			Theorem 3.16			Corollary 3.17		
n	count	Avg	Avg	St.dev	Eq.	Avg	St.dev	Eq.	Avg	St.dev	Eq.	Avg	St.dev	Eq.
3	2	17.0000	17.0000	0.0000	2	17.0000	0.0000	2	17.0000	0.0000	2	17.0000	0.0000	2
4	6	50.3333	50.3138	0.0477	5	50.2000	0.2829	4	50.2690	0.1576	5	50.1225	0.3919	4
5	21	111.8095	111.4828	0.5705	9	111.1203	1.3183	9	111.2337	0.8802	9	110.9713	1.4648	9
6	112	201.6964	200.4406	2.0357	23	199.5614	3.3974	20	199.9065	2.4959	23	199.4028	3.3033	20
7	853	336.5768	333.3367	4.5842	47	331.8240	6.6733	52	332.6419	5.0045	47	332.0414	5.8592	52
8	11117	534.1186	527.3952	8.6967	176	524.9605	11.7328	181	526.9992	8.5569	176	526.2773	9.4637	181
9	261080	824.8016	812.4169	15.0100	657	808.9519	19.1310	890	813.2626	13.3115	657	812.6136	14.1332	890
Theorem 3.19			Lemma 3.21			Lemma 3.22			Lemma 2.5			Lemma 2.6		
Avg	St.dev	Eq.	Avg	St.dev	Eq.	Avg	St.dev	Eq.	Avg	St.dev	Eq.	Avg	St.dev	Eq.
17.0000	0.0000	2	17.0000	0.0000	2	17.0000	0.0000	2	16.5000	0.7071	1	17.0000	0.0000	2
50.0104	0.4687	3	49.7556	0.9205	3	49.8389	0.7455	3	48.1278	3.0493	2	49.9222	0.5894	3
109.9131	2.2811	4	109.4141	3.0841	4	109.4978	2.8112	4	105.5051	7.9455	2	109.5816	2.6621	4
196.3876	6.1267	7	196.4126	6.5589	7	196.0591	6.5432	7	189.3261	15.1541	5	195.7057	6.8659	7
324.9067	13.1437	7	327.0193	11.4814	8	325.3878	12.6381	7	314.6120	25.9379	4	323.7562	14.3586	7
512.8977	23.5953	20	519.1524	17.5357	22	515.2104	21.0413	20	499.3987	39.9663	17	511.2683	25.2940	20
789.8669	38.3841	27	802.7513	25.2540	30	795.2543	32.4719	27	772.7552	58.6286	22	787.7572	40.5713	27

On comparison of the computational results in Tables 5 and 6, we conclude that our lower bounds have the minimum deviation from $F(G)$.

Table 6. Lower bound comparison of $F(G)$ for trees with 10 to 20 vertices.

Parameters			Theorem 3.11			Corollary 3.12			Theorem 3.16			Corollary 3.17		
n	count	Avg	Avg	St.dev	Eq.	Avg	St.dev	Eq.	Avg	St.dev	Eq.	Avg	St.dev	Eq.
10	106	149.3208	148.1451	1.6974	5	146.1565	4.6463	1	146.8356	3.1885	5	143.7363	7.2183	1
11	235	169.0043	167.3584	2.2837	5	164.9952	5.6371	1	165.6850	4.1220	5	112.4892	8.5094	1
12	551	187.7241	185.5305	2.8834	6	182.6395	7.1299	1	183.4392	5.1436	6	179.3669	10.2600	1
13	1301	206.3290	203.5292	3.5690	6	200.2395	8.3068	1	201.0132	6.2306	6	196.5490	11.7586	1
14	3159	224.8224	221.3761	4.2945	7	217.5854	9.7886	1	218.4147	7.3735	7	213.4805	13.4847	1
15	7741	243.3342	239.2007	5.0639	7	234.9688	11.0999	1	235.7963	8.5489	7	230.4596	15.1024	1
16	19320	261.7963	256.9399	5.8827	8	252.2200	12.5741	1	253.0835	9.7808	8	247.3139	16.8339	1
17	48629	280.3229	274.7084	6.7411	8	269.5262	13.9779	1	270.4030	11.0490	8	264.2288	18.5338	1
18	123867	298.8637	292.4569	7.6395	9	286.7946	15.4650	1	287.7006	12.3601	9	281.1144	20.2878	1
19	317955	317.4439	310.2101	8.5743	9	304.0825	16.9327	1	305.0056	13.7060	9	298.0244	22.0410	1
20	823065	336.0508	327.9564	9.5435	10	321.3607	18.4456	1	322.3043	15.0878	10	314.9320	23.8244	1

Theorem 3.19			Lemma 3.21			Lemma 3.22			Lemma 2.5			Lemma 2.6		
Avg	St.dev	Eq.	Avg	St.dev	Eq.	Avg	St.dev	Eq.	Avg	St.dev	Eq.	Avg	St.dev	Eq.
138.6585	13.24038	1	139.1216	5.821731	1	137.7233	2.939934	1	114.3795	53.5970	0	136.3249	15.9161	1
155.6575	16.8429	1	156.2502	17.23116	2	154.5574	18.2061	1	129.1983	60.7702	0	152.8647	20.0324	1
171.7948	20.34513	1	172.4514	20.93671	1	170.5187	21.9951	1	143.6070	66.6434	0	168.5860	23.9875	1
187.8013	23.89991	1	188.5762	24.67797	1	186.3728	25.82532	1	157.8948	72.0964	0	184.1694	27.9987	1
203.7522	27.33324	1	204.6245	28.29714	1	202.1693	29.52746	1	172.1961	77.0235	0	199.7142	31.8593	1
219.7241	30.72609	1	220.7237	31.85541	2	218.0009	33.17812	1	186.4897	81.7499	0	215.2781	35.6770	1
235.6906	33.99504	1	236.8207	35.26777	2	233.8333	36.68944	1	200.7976	86.2529	0	230.8459	39.3555	1
251.7193	37.20559	1	252.9937	38.60288	1	249.7342	40.1334	1	215.1377	90.6975	0	246.4747	42.9739	1
267.7810	40.32793	1	269.207	41.82485	1	265.6736	43.47517	1	229.5057	95.0794	0	262.1403	46.4975	1
283.8829	43.39296	1	285.4704	44.96908	3	281.6582	46.74989	1	243.8976	99.4433	0	277.8459	49.9622	1
300.0174	46.39756	1	301.7732	48.03107	1	297.6795	49.95323	1	258.3142	103.7952	0	293.5857	53.3638	1

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