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, \( \Delta, \Delta_2, \) and \( \delta \) 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

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

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

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

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

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

The first and second Zagreb indices are successfully used in the investigation of the structure-dependency of the total $\pi$-electron energy ($\varepsilon$). It was found that ($\varepsilon$) 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 ($\varepsilon$).

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 $M_1^1(G)$ and forgotten topological index $M_1^2(G)$, 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 $\Delta$ or $\delta$ with $\Delta > \delta \geq 1$. Let $\Gamma$ be the class of graphs such that $d(v_i) = \delta$, $2 \leq i \leq n$. Note that $\Gamma$ is a special case of the bidegreed graphs. Let $\Omega$ 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 $\Theta$ 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 $\Gamma$ and $\Theta$ 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

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

(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 $\alpha$ is a positive number, then

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

(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

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

(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,
\[
F(G) \geq \frac{(M_1(G))^2}{2m} \geq \frac{M_1(G)\cdot 4m^2}{2m} \cdot \left(\frac{2m}{n}\right) = \left(\frac{2m}{n}\right) M_1(G).
\]
Furthermore, the lower bound (2.5) is always better than (2.3):
\[
F(G) \geq \frac{(M_1(G))^2}{m} - 2M_2(G) \geq \left(\frac{4m^2}{n}\right)^2 - 2M_2(G) = \frac{16m^3}{n^2} - 2M_2(G).
\]

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
\[
\Phi^*_1 = \frac{\left[ M_1(G) - \Delta^2 - \Delta_2^2 \right]^2 + (2m - \Delta - \Delta_2) \left( ID(G) - \frac{1}{\Delta} - \frac{1}{\Delta_2} \right) - (n - 2)^2}{(2m - \Delta - \Delta_2)}.
\]
\textbf{Proof} Consider } \omega_1, \omega_2, \ldots, \omega_r \text{ to be the nonnegative weights; then we have the weighted version of the Cauchy–Schwartz inequality: }
\sum_{i=1}^{r} \omega_i a_i^2 \sum_{i=1}^{r} \omega_i b_i^2 \geq \left( \sum_{i=1}^{r} \omega_i a_i b_i \right)^2. \tag{3.2}
\text{Since } \omega_i \text{ is nonnegative, we assume that } \omega_i = x_i - y_i \text{ such that } x_i \geq y_i \geq 0. \text{ 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}
\text{By our assumption, } G \text{ has no isolated vertices and so we have } \frac{1}{d(v)} \leq 1, \text{ for all } v \in V(G). \text{ 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), \text{ and } b_i = 1, \text{ for all } i = 1, 2, \ldots, r \text{ in the above, we get }
\sum_{i=3}^{n} d(v_i)^3 - \left( \sum_{i=3}^{n} d(v_i) \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.
\text{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 \text{ and } \sum_{i=3}^{n} \frac{1}{d(v_i)} = ID(G) - \frac{1}{\Delta} - \frac{1}{\Delta_2} \tag{3.5}
\text{completes the proof. } \square
\text{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), \text{ and } b_i = 1 \text{ in (3.3) for all } i = 1, 2, \ldots, r, \text{ we have the following result.}
\textbf{Corollary 3.2} \text{ With the assumptions in Theorem 3.5, one has the inequality }
F(G) \geq \Delta^3 + \Delta^2 + \Phi_2^* \tag{3.6}
\text{with equality if and only if } G \text{ is regular or } G \in \Gamma \text{ or } G \in \Theta, \text{ where }
\Phi_2^* = \frac{[M_1(G) - \Delta^2 - \delta^2]^2 + (2m - \Delta - \delta) (ID(G) - \frac{1}{\Delta} - \frac{1}{\Delta_2}) - (n - 2)^2}{(2m - \Delta - \delta)}.
\textbf{Remark 3.3} \text{ 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) \text{ and } W(t, 7) - v_n, \text{ other than the equality case.}
\text{By setting } x_i = d(v_i), \ y_i = 0, \ a_i = d(v_i), \text{ and } b_i = 1 \text{ in (3.3) immediately has (2.4) as its special case.}
\text{Also, by comparing the choice of selection of } y_i \text{ 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.}
Remark 3.4 The lower bounds (3.1) and (3.6) are incomparable. Namely, there exists a molecular graph of 1,2-diethylocyclopentane for which (3.1) is better than (3.6) and there exists a molecular graph of 1,1-diethylocyclopentane 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

\[
F(G) \geq \Delta^3 + \Delta^3_2 + \Phi^*_3
\]

(3.7)

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

\[
\Phi^*_3 = \left( M_1(G) - \Delta^2 - \Delta^2_2 \right)^2 + (n-2) \left( M_1(G) - \Delta^2 - \Delta^2_2 \right) - (2m - \Delta - \Delta_2) .
\]

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. \qed
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
\[
F(G) \geq \Delta^3 + \delta^3 + \Phi_4^*
\]  
with equality if and only if \( G \) is regular or \( G \in \Gamma \) or \( G \in \Theta \), where
\[
\Phi_4^* = \frac{(M_1(G) - \Delta^2 - \delta^2)^2 + (n - 2) (M_1(G) - \Delta^2 - \delta^2)}{(2m - \Delta - \delta)} - (2m - \Delta - \delta).
\]

**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
\[
\Phi_5^* \geq \Phi_1^*, \Phi_4^* \geq \Phi_2^*.
\]
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
\[
(M_1(G) - \Delta^2 - \Delta_2^2) (n - 2) - (2m - \Delta - \Delta_2)^2 \\
\geq (2m - \Delta - \Delta_2) \left( ID(G) - \frac{1}{\Delta} - \frac{1}{\Delta_2} \right) - (n - 2)^2.
\]
Adding \((M_1(G) - \Delta^2 - \Delta_2^2)^2\) and dividing by \( (2m - \Delta - \Delta_2) \) on both sides of the above inequality completes our claim of \( \Phi_5^* \geq \Phi_1^* \). In an analogous manner we complete our second claim.

Intuitively one may conjecture that \( \Phi_5^* \geq \Phi_1^* \) and \( \Phi_4^* \geq \Phi_2^* \). 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
\[
F(G) \geq \Delta^3 + \Delta_2^3 + \Upsilon^*_1
\]  
with equality if and only if \( G \) is regular or \( G \in \Gamma \) or \( G \in \Omega \), where
\[
\Upsilon^*_1 = \frac{(M_1(G) - \Delta^2 - \Delta_2^2) + \sqrt{(2m - \Delta - \Delta_2) \left( ID(G) - \frac{1}{\Delta} - \frac{1}{\Delta_2} \right) - (n - 2)^2}}{(2m - \Delta - \Delta_2)}.
\]

**Proof** Consider \( w_1, w_2, \ldots, w_r \) to be the nonnegative weights; then, from (3.2), we have
\[
\left( \sum_{i=1}^{r} w_i a_i^2 \right)^{\frac{1}{2}} \left( \sum_{i=1}^{r} w_i b_i^2 \right)^{\frac{1}{2}} \geq \sum_{i=1}^{r} w_i a_i b_i.
\]
Since \( w_i \) is nonnegative, we assume that \( w_i = x_i - y_i \) such that \( x_i \geq y_i \geq 0 \). Thus,
\[
\left( \sum_{i=1}^{r} x_i a_i \right)^{\frac{1}{2}} \left( \sum_{i=1}^{r} x_i b_i \right)^{\frac{1}{2}} - \sum_{i=1}^{r} x_i a_i b_i \geq \left( \sum_{i=1}^{r} y_i a_i \right)^{\frac{1}{2}} \left( \sum_{i=1}^{r} y_i b_i \right)^{\frac{1}{2}} - \sum_{i=1}^{r} y_i a_i b_i \geq 0.
\] (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
\[
F(G) \geq \Delta^3 + \delta^3 + \Upsilon_2^*
\] (3.12)
with equality if and only if \( G \) is regular or \( G \in \Gamma \) or \( G \in \Theta \), where
\[
\Upsilon_2^* = \left( (M_1(G) - \Delta^2 - \delta^2) + \sqrt{(2m - \Delta - \delta) (ID(G) - \frac{1}{\Delta} - \frac{1}{\Delta_2}) - (n - 2)} \right)^2
\]
\[
\quad \quad \frac{2m - \Delta - \Delta_2}{(2m - \Delta - \delta)}.
\]

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

Adding \( (M_1(G) - \Delta^2 - \Delta_2^2)^2 + (2m - \Delta - \Delta_2) (ID(G) - \frac{1}{\Delta} - \frac{1}{\Delta_2}) \) 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, \( \Upsilon_1^* \) and \( \Upsilon_2^* \) 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>
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<th>( Fl_{15} )</th>
<th>( T_2(Fl_{15}) )</th>
<th>( L(Fl_{15}) )</th>
<th>( T_1[L(Fl_{15})] )</th>
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<td>91</td>
<td>60</td>
<td>600</td>
</tr>
<tr>
<td>( m )</td>
<td>60</td>
<td>660</td>
<td>540</td>
<td>1620</td>
</tr>
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<td>( F(G) )</td>
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<td>900720</td>
<td>7210080</td>
</tr>
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<td>(3.9)</td>
<td>28013.501</td>
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<td>4016746.829</td>
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<td>(3.12)</td>
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<td>817804.321</td>
<td>4571543.636</td>
</tr>
</tbody>
</table>
Theorem 3.11 Let $G$ be a simple graph of order $n (\geq 3)$. Then

$$F(G) \geq \Delta^3 + \Delta^2 + \Upsilon_3^*$$

(3.13)

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

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

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 $i = 1, 2, \cdots , r$. \hfill \Box

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

$$F(G) \geq \Delta^3 + \delta^3 + \Upsilon_4^*$$

(3.14)

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

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

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

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

(3.15)

It is easy to see that

$$(M_1(G) - \Delta^2 - \Delta_2^2) \geq (2m - \Delta - \Delta_2).$$  

(3.16)

By multiplying (3.15) and (3.16), then by adding the terms $(n-2)(M_1(G) - \Delta^2 - \Delta_2^2)$ and $(M_1(G) - \Delta^2 - \Delta_2^2)^2$, 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 $\Upsilon_1^* \geq \Phi_3^*$ and $\Upsilon_2^* \geq \Phi_4^*$. 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).

<table>
<thead>
<tr>
<th></th>
<th>$H_6$</th>
<th>$L(H_6)$</th>
<th>$L(H_6)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n$</td>
<td>13</td>
<td>18</td>
<td>18</td>
</tr>
<tr>
<td>$m$</td>
<td>18</td>
<td>51</td>
<td>102</td>
</tr>
<tr>
<td>$F(G)$</td>
<td>606.0</td>
<td>4530.0</td>
<td>28824.0</td>
</tr>
<tr>
<td>(3.9)</td>
<td>582.805</td>
<td>4257.69</td>
<td>28129.816</td>
</tr>
<tr>
<td>(3.7)</td>
<td>574.846</td>
<td>4253.023</td>
<td>28129.909</td>
</tr>
</tbody>
</table>

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

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

(3.17)

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

(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

$$F(G) = \chi^2(G) - 2\sigma_G (P_4) - 4\sigma_G (P_5) - 6\sigma_G (C_3) - 2m.$$  

From [16], we have

$$M_1(G) \geq \Delta^2 + \Delta_2^2 + \Psi_1^*, \quad M_1(G) \geq \Delta^2 + \delta^2 + \Psi_2^*,$$

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

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

(3.19)

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

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

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

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

(3.20)

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

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

Remark 3.18 In [16], the present authors proved that $\Psi_1^*$ and $\Psi_2^*$ 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).

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th>(F(G))</th>
<th>(3.19)</th>
<th>(3.20)</th>
<th>(3.13)</th>
<th>(3.14)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(W(2, 15))</td>
<td>46</td>
<td>75</td>
<td>5310</td>
<td>5228.3</td>
<td>5235.443</td>
<td>5295.659</td>
<td>5297.542</td>
</tr>
<tr>
<td>(T_1(W(2, 15)))</td>
<td>121</td>
<td>225</td>
<td>43080</td>
<td>41192.289</td>
<td>41155.235</td>
<td>40548.176</td>
<td>40541.287</td>
</tr>
<tr>
<td>(T_2(W(2, 15)))</td>
<td>121</td>
<td>435</td>
<td>133110</td>
<td>126445.071</td>
<td>126136.04</td>
<td>107890.171</td>
<td>106750.598</td>
</tr>
</tbody>
</table>

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

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

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

\[
\sum_{uv \in E(G)} (d(u) + d(v))^2 \sum_{uv \in E(G)} 1 - \left(\sum_{uv \in E(G)} (d(u) + d(v))\right)^2 \\
\geq \sum_{uv \in E(G)} 2\left(d(u) + d(v)\right) \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)} - \left(\sum_{uv \in E(G)} 1\right)^2 \\
(F(G) + 2M_2(G)) m - (M_1(G))^2 \geq 2M_1(G)H(G) - 4m^2,
\]

which completes the proof. \(\Box\)

**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

\[
F(G) \geq \frac{\text{irr}^2(G)}{m} + 2M_2(G),
\]

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

\[
F(G) \geq \frac{\text{irr}^2(G) + M_1(G)^2}{2m},
\]

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.

<table>
<thead>
<tr>
<th></th>
<th>( F(G) )</th>
<th>(3.19)</th>
<th>(3.20)</th>
<th>(3.13)</th>
<th>(3.14)</th>
<th>(3.21)</th>
<th>(3.22)</th>
<th>(3.23)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_{r6} )</td>
<td>168</td>
<td>155.948</td>
<td>157.282</td>
<td>163.984</td>
<td>165.082</td>
<td>158</td>
<td>156</td>
<td>156</td>
</tr>
<tr>
<td>( L(C_{r6}) )</td>
<td>432</td>
<td>413.096</td>
<td>413.029</td>
<td>415.135</td>
<td>416.240</td>
<td>417.333</td>
<td>416</td>
<td>416</td>
</tr>
<tr>
<td>( T_1(C_{r6}) )</td>
<td>1440</td>
<td>1317.589</td>
<td>1297.954</td>
<td>1275.261</td>
<td>1262.972</td>
<td>1264</td>
<td>1312</td>
<td>1280</td>
</tr>
<tr>
<td>( T_2(C_{r6}) )</td>
<td>1848</td>
<td>1757.666</td>
<td>1755.619</td>
<td>1760.189</td>
<td>1752.480</td>
<td>1675.205</td>
<td>1800</td>
<td>1731.429</td>
</tr>
</tbody>
</table>

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 \( \alpha \geq 1 \),

\[
M^{\alpha+1}(G) = (n - 1)M^\alpha(G) - M^{\alpha+1}(G).
\]

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 \( \Delta \), second maximum degree \( \Delta_2 \), and minimum degree \( \delta \). Then

\[
\mathcal{F}(G) \leq (n - 1)M_1(G) - [\Delta^3 + \Delta_2^3 + \Psi_3^*]
\]

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

\[
\mathcal{F}(G) \leq (n - 1)M_1(G) - [\Delta^3 + \delta^3 + \Psi_4^*]
\]

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 \( \Delta \), second maximum degree \( \Delta_2 \), and minimum degree \( \delta \). Then

\[
\mathcal{F}(G) \geq (n - 1) [\Delta^2 + \Delta_2^2 + \Psi_3^*] - F(G)
\]

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

\[
\mathcal{F}(G) \geq (n - 1) [\Delta^2 + \delta^2 + \Psi_3^*] - F(G)
\]

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:

\[
F(G) + F(\overline{G}) \geq \frac{n(n - 1)^3}{4}.
\]

Now we give new lower bounds on \( F(G) + F(\overline{G}) \) in terms of \( n, m, \Delta, \delta \), and \( ID(G) \).
Theorem 3.27 Let $G$ be a simple graph with $n$ nonisolated vertices, $m$ edges, maximum degree $\Delta$, second maximum degree $\Delta_2$, and minimum degree $\delta$. Then

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

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

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

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

Proof It is easy to see that

$$F(\overline{G}) = \sum_{i=1}^{n} (n - 1 - d_G(v_i))^3$$

$$= n(n-1)^3 - 6m(n-1)^2 + 3(n-1)M_1(G) - F(G).$$

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. \hfill \Box

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 $\overline{F}(G) + F(\overline{G})$.

Corollary 3.28 Let $G$ be a simple graph with $n$ nonisolated vertices, $m$ edges, maximum degree $\Delta$, second maximum degree $\Delta_2$, and minimum degree $\delta$. Then

$$\overline{F}(G) + F(\overline{G}) \geq n(n-1)^3 - 4m(n-1)^2 - [F(G) + F(\overline{G})]$$

$$+ 2(n-1)(\Delta^2 + \Delta_2^2 + \Psi_1^*)$$

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

$$\overline{F}(G) + F(\overline{G}) \geq n(n-1)^3 - 4m(n-1)^2 - [F(G) + F(\overline{G})]$$

$$+ 2(n-1)(\Delta^2 + \delta^2 + \Psi_2^*)$$

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. \hfill \Box

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
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, and the number of graphs holding equality.

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

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Theorem 3.11</th>
<th>Corollary 3.12</th>
<th>Theorem 3.16</th>
<th>Corollary 3.17</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n )</td>
<td>( \text{count} )</td>
<td>Avg</td>
<td>St.dev</td>
<td>Eq</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>17.0000</td>
<td>0.0000</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>6</td>
<td>50.3333</td>
<td>0.0477</td>
<td>5</td>
</tr>
<tr>
<td>5</td>
<td>21</td>
<td>111.8095</td>
<td>0.5705</td>
<td>9</td>
</tr>
<tr>
<td>6</td>
<td>112</td>
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<td>2.0357</td>
<td>23</td>
</tr>
<tr>
<td>7</td>
<td>853</td>
<td>336.5768</td>
<td>4.5842</td>
<td>47</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Theorem 3.11</th>
<th>Corollary 3.12</th>
<th>Theorem 3.16</th>
<th>Corollary 3.17</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n$</td>
<td>Avg</td>
<td>St.dev</td>
<td>Eq</td>
<td>Avg</td>
</tr>
<tr>
<td>10</td>
<td>149.3208</td>
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</tr>
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<td>5</td>
</tr>
<tr>
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<td>2.8834</td>
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</tr>
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<td>3.5000</td>
<td>6</td>
</tr>
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<td>221.3761</td>
<td>4.2945</td>
<td>7</td>
</tr>
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<td>7</td>
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<td>19</td>
<td>317.4380</td>
<td>310.2101</td>
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<td>9</td>
</tr>
<tr>
<td>20</td>
<td>320.6508</td>
<td>327.5644</td>
<td>9.5445</td>
<td>10</td>
</tr>
</tbody>
</table>

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References


