On reformulated zagreb indices with respect to tricyclic graphs

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Abstract

The authors Miličević et al. introduced the reformulated Zagreb indices \cite{20}, which is a generalization of classical Zagreb indices of chemical graph theory. In the paper, we characterize the extremal properties of the first reformulated Zagreb index. We first introduce some graph operations which increase or decrease this index. Furthermore, we will determine the extremal tricyclic graphs with minimum and maximum the first Zagreb index by these graph operations.

Keywords: The reformulated Zagreb index, Zagreb indices, Tricyclic graph, edge degree, Graph operation

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1 Introduction

Topological indices are major invariants to characterize some properties of the graph of a molecule. One of the most important topological indices is the well-known Zagreb indices, as a pair of molecular descriptors, introduced in \cite{14,23}. For a simple graph $G$, the first and second Zagreb indices, $M_1$ and $M_2$, respectively, are defined as:

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

Zagreb indices, as a pair of molecular descriptors, first appeared in the topological formula for the total - energy of conjugated molecules that has been derived in 1972 \cite{14}. Soon

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after these indices have been used as branching indices \[13\]. Later the Zagreb indices found applications in QSPR and QSAR studies \[1, 9, 23\].

Since an edge of graph \(G\) transform to a corresponding vertex of the line graph \(L(G)\). Motivated by the connection, Milićević et al. \[20\] in 2004 reformulated the Zagreb indices in terms of edge-degrees instead of vertex-degrees as:

\[
EM_1(G) = \sum_{e \in E} \text{deg}(e)^2, \quad EM_2(G) = \sum_{e \sim f} \text{deg}(e) \cdot \text{deg}(f),
\]

where \(\text{deg}(e)\) denotes the degree of the edge \(e\) in \(G\), which is defined as \(\text{deg}(e) = \text{deg}(u) + \text{deg}(v) - 2\) with \(e = uv\), and \(e \sim f\) means that the edges \(e\) and \(f\) are adjacent, i.e., they share a common end-vertex in \(G\).

In order to exhibit our results, we introduce some graph-theoretical notations and terminology. For other undefined ones, see the book \[2\].

Let \(S_n, P_n, C_n\) be the star, path and cycle on \(n\) vertices, respectively. Let \(G = (V; E)\) be a simple undirected graph. For \(v \in V(G)\) and \(e \in E(G)\), let \(N_G(v)\) (or \(N(v)\) for short) be the set of all neighbors of \(v\) in \(G\), \(G - v\) be a subgraph of \(G\) by deleting vertex \(v\), and \(G - e\) be a subgraph of \(G\) by deleting edge \(e\). Let \(G_0\) be a nontrivial graph and \(u\) be its vertex. If \(G\) is obtained by \(G_0\) fusing a tree \(T\) at \(u\). Then we say that \(T\) is a subtree of \(G\) and \(u\) is its root. Let \(uv\) denote the fusing two vertices \(u\) and \(v\) of \(G\). Let \(S_n^m\) denote the graph obtained by connecting one pendent to \(m - n + 1\) others pendents of \(S_n\). In addition, we replace the sign “if and only if” by “iff” for short.

Recently, the upper and lower bounds on \(EM_1(G)\) and \(EM_2(G)\) were presented in \[7, 18, 34\]; Su et al. \[22\] characterize the extremal graph properties on \(EM_1(G)\) with respect to given connectivity. As some examples, we now introduce the extremal of \(EM_1(G)\) among acyclic, unicyclic, bicyclic graphs, respectively.

**Theorem 1.1** Let \(G\) be a acyclic connected graph with order \(n\). Then

\[
EM_1(P_n) \leq EM_1(G) \leq EM_1(S_n),
\]

while the lower bound is attached iff \(G \cong P_n\) and the upper bound is attached iff \(G \cong S_n\).

Ilić and Zhou \[18\] obtained the next conclusion. Ji and Li \[19\] provided a shorter proof by utilizing some graph operations.

**Theorem 1.2** Let \(G\) be a unicyclic graph with \(n\) vertices. Then

\[
EM_1(C_n) \leq EM_1(G) \leq EM_1(S_n^m),
\]

while the lower bound is attached iff \(G \cong C_n\) and the upper bound is attached iff \(G \cong S_n^m\).

In \[19\], the authors also got the bound of \(EM_1\) among bicyclic graphs and completely characterized the extremal graphs correspondingly.
Theorem 1.3  Let $G$ be a bicyclic graph with $n$ vertices. Then
\[4n + 34 \leq EM_1(G) \leq n^3 - 5n^2 + 16n + 4,\]
where the lower bound is attached iff $G \in \{P_n^{k,l,m} : \ell \geq 3\} \cup \{C_n(r, \ell, t) : \ell \geq 3\}$ and the upper bound is attached iff $G \cong S_n^{n+1}$.

The latest related results on $EM_1$ refer to [6,10,11,26,29].

In this paper we characterize the extremal properties of the first reformulated Zagreb index. In Section 2 we present some graph operations which increase or decrease $EM_1$. In Section 3, we determine the extremal tricyclic graphs with minimum and maximum the first Zagreb index.

2 Some graph operations

In the section we will introduce some graph operations, which increase or decrease the first reformulated Zagreb index. In fact, these graph operations will play a key role in determining the extremal graphs of the first reformulated Zagreb index among all tricyclic graphs.

Now we introduce two graph operations [19] which strictly increases the first reformulated Zagreb index of a graph.

Operation I. As shown in Fig. 1, let $uv$ be an edge of connected graph $G$ with $d_G(v) \geq 2$. Suppose that $\{v, w_1, w_2, \ldots, w_t\}$ are all the neighbors of vertex $u$ while $w_1, w_2, \ldots, w_t$ are pendent vertices. If $G' = G - \{uw_1, uw_2, \ldots, uw_t\} + \{vw_1, vw_2, \ldots, vw_t\}$, we say that $G'$ is obtained from $G$ by Operation I.

![Fig. 1 Graphs $G$ and $G'$ in Operation I.](image)

Operation II. As shown in Fig. 2, Let $G$ be nontrivial connected graph $G$ and $u$ and $v$ be two vertices of $G$. Let $P_\ell = v_1(=u)v_2\cdots v_\ell(=v)$ is a nontrivial $\ell$-length path of $G$ connecting vertices $u$ and $v$. If $G' = G - \{v_1v_2, v_2v_3, \ldots, v_{\ell-1}v_\ell\} + \{w(=u \circ v)v_1, wv_2, \ldots, wv_\ell\}$, we say that $G'$ is obtained from $G$ by Operation II.

![Fig. 2 The graphs $G$ and $G'$ in Operation II.](image)
In fact, those inverse operation of Operation I and Operation II decrease $EM_1$ of a graph. According the above two graph operations, it is immediate to get the following two results [19].

Lemma 2.1 If $G'$ is obtained from $G$ by Operation I as shown in Fig. 1, then

$$EM_1(G) < EM_1(G').$$

Lemma 2.2 If $G'$ is obtained from $G$ by Operation II as shown in Fig. 2, then

$$EM_1(G) < EM_1(G').$$

Operation III. As shown in Fig. 3, let $G_0$ be a nontrivial subgraph(acyclic) of $G$ with $|G_0| = t$ which is attached at $u_1$ in graph $G$, $x$ and $y$ be two neighbors of $u_1$ different from in $G_0$. If $G' = G - (G_0 - u_1) + u_1v_2 + v_2v_3 + \cdots + v_y$, we say that $G'$ is obtained from $G$ by Operation III.

Fig. 3 Graphs $G$, $G'$, $G_1$ in Operation III.

Lemma 2.3 Let $G$ and $G'$ be two graphs as shown in Fig. 3. Then we have

$$EM_1(G) > EM_1(G')$$

Proof. According to the inverse of Operation I, as shown in Fig. 3, there is a graph $G_1$ such that $EM_1(G) \geq EM_1(G_1)$. In order to show the conclusion, we now just to verify the following Inequality:

$$EM_1(G_1) > EM_1(G').$$

(2.1)

By means of the definition of $EM_1$, we have

$$EM_1(G) - EM_1(G') > d_{G_1}^2(u_1u_2) + d_{G_1}^2(u_1v) + d_{G_1}^2(u_{t-1}u_t) - [d_{G'}^2(u_1u_2) + d_{G'}^2(u_{t-1}u_t) + d_{G'}^2(u_tv)]$$

$$= d_{G_1}^2(u_1) + (d_{G_1}(u_1) + d_{G_1}(v))^2 - (d_{G_1}(u_1) - 1)^2 - d_{G_1}(v) - 1.$$

$$= d_{G_1}^2(u_1) + 2d_{G_1}(u_1)d_{G_1}(v) + 2d_{G_1}(u_1) - 2 > 0$$

Therefore, the Ineq. (2.1) holds. Then we finish the proof.

Operation IV. Let $G_0$ be a nontrivial connected graph and $u$ and $v$ are two vertices in $G_0$ with $d_{G_0}(u) = x, d_{G_0}(v) = y$ and $N_{G_0}(u) \supset N_{G_0}(v)$. Let $G$ be the graph obtained by attaching $S_k+1$ and $S_{t+1}$ at the vertices $u$ and $v$ of $G_0$, respectively. If $G'$ is the graph obtained by delating the $\ell$ pendant vertices at $v$ in $G$ and connecting them to $u$ of $G$, depicted in Fig. 4, We say that $G'$ is obtained from $G$ by Operation IV.
Fig. 4 \( G \) and \( G' \) in Operation IV.

Lemma 2.4 If \( G' \) is obtained from \( G \) by Operation V as shown in Figure 4. Then

\[
EM_1(G) < EM_1(G').
\]

Proof. Note that \( d_{G_0}(u) = x \), and \( d_{G_0}(v) = y > 0 \), meanwhile \( N_{G_0}(u) \supseteq N_{G_0}(v) \). By the definition of \( EM_1 \), we have

\[
\begin{align*}
EM_1(G') - EM_1(G) &> \sum_{i=1}^{k} [d_{G'}^2(uu_i) - d_{G}^2(uu_i)] + \sum_{i=1}^{\ell} [d_{G'}^2(uv_i) - d_{G}^2(uv_i)] \\
&+ \sum_{w \in N_{G_0}(v)} [d_{G'}^2(uw) + d_{G}^2(uw)] - \sum_{w \in N_{G_0}(v)} [d_{G'}^2(uw) + d_{G}^2(uw)] \\
&= (k + \ell)(k + \ell + x - 2)^2 - k(k + x - 2)^2 - \ell(\ell + y - 2)^2 \\
&+ \sum_{w \in N_{G_0}(v)} [(k + \ell + x - d_{G_0}(w) - 2)^2 + (y + d_{G_0}(w) - 2)^2] \\
&- \sum_{w \in N_{G_0}(v)} [(k + x + d_{G_0}(w) - 2)^2 + (\ell + y + d_{G_0}(w) - 2)^2] \\
&> 2\ell(x + k - y) > 0.
\end{align*}
\]

So the result follows. \( \blacksquare \)

As the above exhibited, Operation III strictly decrease the \( EM_1 \) of a graph; while all of Operation I, Operation II and Operation IV strictly increase the \( EM_1 \) of a graph.

3 Main results

In the section, we will characterize the extremal graph with respect to \( EM_1 \) among all tricyclic graphs by some graph operations.

For convenience, let define some notations which will be using in the sequel. Denote by \( \mathcal{C}_n \) the set of all connected tricyclic graphs with order \( n \). For any tricyclic graph \( G \), the subgraph which is obtained by deleting all pendent of \( G \) is referred as a brace of \( G \). Let \( \mathcal{C}_{n}^{0} \) be the set of all braces of tricyclic graphs as pictured in Fig. 5, and \( \mathcal{C}_n^{1} \) denote the set of these tricyclic graphs shown in Fig. 6. Moreover, \( \mathcal{C}_n^{2} \) denote the set of these tricyclic graphs depicted in Fig. 7.

Fig. 5 The graphs in \( \mathcal{C}_n^{1} \)

Fig. 6 The graphs in \( \mathcal{C}_n^{2} \)

Fig. 7 Some graphs using in the later proof.

We next introduce the extremal graphs with respect to \( EM_1 \) on tricyclic graphs.
Theorem 3.1 Let $G$ be a tricyclic graph with order $n$. Then

$$4n + 68 \leq EM_1(G),$$

where the equality holds iff $G \in \mathcal{C}_n^1$.

Proof. Let $G$ be a connected tricyclic graph. By Lemma 2.2, $G$ can be converted to the one of the fifteen graphs without any pendant as shown in Fig. 5. In other words, there exists a graph $\alpha_i \in \mathcal{C}_n^0$ ($i \leq 15$) such that $EM_1(G) \geq EM_1(\alpha_i)$ in terms of Lemma 2.3 for any given graph $G$. By directed calculation, we obtain that

$$EM_1(\beta_i) = 4n + 68, \text{ for } i = 1, 2, \cdots, 5.$$

Then the proof complete.

Theorem 3.2 Let $G$ be a tricyclic graph with order $n$. Then

$$EM_1(G) \leq n^3 - 5n^2 + 20n + 32,$$

where the equality holds iff $G \cong S_n^{n+2}$ or $S_n^{K_4}$.

Proof. For a given connected tricyclic graph $G$, with repeated Operation II and Operation IV, it can be converted to the one of the five graphs as shown in Fig. 6. That is to say, For any tricyclic graph $G$ with order $n$, there exists $\gamma_i \in \mathcal{C}_n^2$ ($i \leq 6$) such that $EM_1(G) \leq EM_1(\gamma_i)$ in views of Lemma 2.2 and Lemma 2.4.
By indirected calculating, we get

\[ EM_1(\gamma_1) = n^3 - 5n^2 + 16n + 18, \quad EM_1(\gamma_2) = n^3 - 5n^2 + 20n - 10, \]
\[ EM_1(\gamma_3) = n^3 - 5n^2 + 20n + 2, \quad EM_1(\gamma_4) = n^3 - 9n^2 + 32n + 60, \]
\[ EM_1(S^{3}_n) = n^3 - 5n^2 + 20n + 32, \quad EM_1(S^{K_4}_n) = n^3 - 5n^2 + 20n + 32. \]

Therefore we complete the proof. \[ \square \]

Together Theorem 3.1 with Theorem 3.2, the main result is shown.

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