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The reformulated Zagreb indices of tricyclic graphs

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ABSTRACT

Miličević et al. first introduced the reformulated Zagreb indices, which is a generalization of classical Zagreb indices of chemical graph theory. As we know, the Zagreb indices have been found applications in QSPR and QSAR studies. In the paper, we characterize the extremal properties of the first reformulated Zagreb index. We show some graph operations which increase or decrease this index. Furthermore, we determine the sharp bound of the first reformulated Zagreb index among all the extremal tricyclic graphs by these graph operations.

1. Introduction

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 $u \circ v$ denote the fusing two vertices u and v of G. Let S_n, P_n and C_n be the star, path and cycle on n vertices, respectively. Let S_n^m denote the graph obtained by connecting one pendent to $m - n + 1$ other pendents of S_n. For other undefined notations and terminology, see the book [6]. In addition, we replace the sign "if and only if" by "iff" for short.

A graph invariant is a number related to a graph which is a structural invariant, that is, it is a fixed number under graph automorphism. In chemical graph theory, these invariants are also referred to as the topological indices, which 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 [18,38]. For a simple graph G, the first and second Zagreb indices, M_1 and M_2, respectively, are defined as:

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

Zagreb indices, first appeared in the topological formula for the total π-energy of conjugated molecules that has been derived in 1972 [18]. Soon after these indices have been used as branching indices [17]. Later the Zagreb indices found applications in QSPR and QSAR studies [5,9,38]. This theory is developed well (see reviews [14,35]), the latest results may be found in a number of literatures [1–4,7,12,13,15,19,20,22,23,27,32,39,40,42] and the references cited therein. In fact, the first Zagreb index is a special version of zeroth order Randic index [16,21,30]. There are also many other topological indices are studied [10,11,26,28,29,31,33,36,41].

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Fig. 1. Graphs G and G' in Operation I.

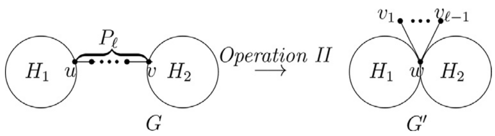

Fig. 2. The graphs G and G' in Operation II.

Since an edge of graph G corresponds to a vertex of the line graph $L(G)$. Motivated by the connection, Miličević et al. [34] in 2004 reformulated the Zagreb indices in terms of edge-degrees instead of vertex-degrees as:

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

where $\deg(e)$ denotes the *degree of the edge* e in G, which is defined as $\deg(e) = \deg(u) + \deg(v) - 2$ 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.

Recently, the upper and lower bounds on $EM_1(G)$ and $EM_2(G)$ were presented in [8,24,43]; Su et al. [37] characterize the extremal graph properties on $EM_1(G)$ with a given connectivity $\mathcal{K}$. As some examples, we next introduce the extremal-value of $EM_1(G)$ among acyclic, unicyclic, bicyclic graphs, respectively.

Theorem 1. *Let G be a acyclic connected graph with order n. Then*

$$EM_1(P_n) \le EM_1(G) \le EM_1(S_n),$$

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 [24] obtained the next conclusion. Ji and Li [25] lately provided a shorter proof for it by utilizing some graph operations.

Theorem 2. *Let G be a unicyclic graph with n vertices. Then*

$$EM_1(C_n) \le EM_1(G) \le EM_1(S_n^n),$$

while the lower bound is attached iff $G \cong C_n$ and the upper bound is attached iff $G \cong S_n^n$.

In [25], the authors also got the bound of EM_1 among bicyclic graphs and completely characterized the extremal graphs correspondingly.

Theorem 3. *Let G be a bicyclic graph with n vertices. Then*

$$4n + 34 \le EM_1(G) \le n^3 - 5n^2 + 16n + 4,$$

where the lower bound is attached iff $G \in \{P_n^{k,\ell,m} : \ell \ge 3\} \cup \{C_n(r, \ell, t) : \ell \ge 3\}$ and the upper bound is attached iff $G \cong S_n^{n+1}$.

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 an key role in determining the extremal graphs of the first reformulated Zagreb index among all tricyclic graphs.

Now we introduce two graph operations [25] which strictly increase 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 $d_G(v) \ge 2$. Suppose that $\{v, w_1, w_2, \cdots w_t\}$ are all the neighbors of vertex u while $w_1, w_2, \cdots w_t$ are pendent vertices. If $G' = G - \{uw_1, uw_2, \cdots uw_t\} + \{vw_1, vw_2, \cdots vw_t\}$, we say that G' is obtained from G by *Operation I*.

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 ℓ- length path of G connecting vertices u and v. If $G' = G - \{v_1v_2, v_2v_3, \cdots, v_{\ell-1}v_\ell\} + \{w(= u \circ v)v_1, wv_2, \cdots, wv_\ell\}$, we say that G' is obtained from G by *Operation II*.