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ON THE MAXIMUM AND MINIMUM FIRST REFORMULATED ZAGREB INDEX OF GRAPHS WITH CONNECTIVITY AT MOST k

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Abstract

The authors Miličević et al. introduced the reformulated Zagreb indices [1], which is a generalization of classical Zagreb indices of chemical graph theory. In this paper, we mainly consider the maximum and minimum for the first reformulated index of graphs with connectivity at most k. The corresponding extremal graphs are characterized.

1 Introduction

A graph invariant is a function on a graph that does not depend on the labeling of its vertices. Recently, hundreds of graph invariants have been considered in quantitative structure-activity relationship and quantitative structure-property relationship researches. We refer the reader to the monograph [2]. Among those useful invariants, we will present several that are relevant for our paper, such as the first Zagreb index and the second Zagreb index [3-7].

The authors modified the Zagreb indices in [8]. Later, the Zagreb indices were reformulated in terms of the edge-degrees instead of the vertex-degrees as the original Zagreb indices, named the reformulated Zagreb indices, by Miličević et al. in 2004 [9].

As far as we know, there are only some basic mathematical properties of the reformulated Zagreb indices have been reviewed [9]. Other investigators discussed the relationship between the reformulated Zagreb indices and the corresponding invariants of graphs [10]. Whereas to our best knowledge, the reformulated Zagreb indices with order n and k cut vertices or connectivity at most k have, so far, not been considered in the chemical literatures. The aim of the present article is to continue in the same vein and to give some novel results concerning these indices. Here we mainly consider a special classes of graphs with order n and connectivity at most k. The corresponding extremal graphs are also presented.

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2 Terminology and notations

Throughout the paper we consider only finite and simple graphs. Let $G = (V, E)$ be a finite simple graph with vertex set V and edge set E, and $|G|$ and $|E|$ be its order and size, respectively. As usual, the *degree* of a vertex u in G is the number of incident edges, denoted by $d_G(u)$ or $d(u)$ for short if there is no confuse, and the *neighborhood* of a vertex u in G is denoted by $N_G(u)$ or $N(u)$ for short. The *complement* of G, denoted by $\overline{G}$, is a simple graph on the same set of vertices $V(G)$, in which two vertices u and v are adjacent if and only if they are not adjacent in G. For simplicity, we let $m = |E|$ and $\overline{m} = |\overline{E}|$, hence $\overline{m} + m = \binom{n}{2}$ and the degree of the same vertex u in $\overline{G}$ is then given by $d_{\overline{G}}(u) = n-1-d_G(u)$, respectively.

The first Zagreb index M_1 equals to the sum of squares of the vertex degrees, and the second Zagreb index M_2 equals to the sum of product of degree of pairs of adjacent vertices:

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

We refer the reader to [4] for more information and results on Zagreb indices.

In 2004, Miličević, Nikolić and Trinajstić reformulated the Zagreb indices in terms of edge-degrees instead of vertex-degrees [1]:

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

where $d(e) = d(u) + d(v) - 2$ denotes the degree of the edge e in G, and $e \sim f$ means that the edges e and f share a common end-vertex in G.

Let G be a graph, then $G + uv$ denotes the graph obtained from G by adding an edge uv for two non-adjacent vertices u and v. Similarly, $G - uv$ denotes the graph obtained by deleting an edge uv of G.

A subgraph obtained by vertex deletions only is said to be an *induced subgraph*. If S is the set of deleted vertices, the resulting subgraph is denoted by $G - S$. If $T = V \setminus S$, in this case, the subgraph is denoted by $G[T]$ and referred to as the subgraph of G induced by T. We call T is a *clique* if the induced subgraph $G[T]$ is complete.

A *cut-vertex* in a connected graph G is a vertex whose deletion breaks the graph into at least two connected components, and a *vertex-cut* of a graph G is a set X of $V(G)$ such that $G - X$ has more than one component. Similarly, the *edge-cut* Y of graph G is a set of edges such that $G - Y$ has more than one component.

The *connectivity* of G, denoted by $\kappa(G)$, is the minimum size of a vertex set R such that $G - R$ is disconnected or has only one vertex. A graph G is *k-connected* if its connectivity is at least k. The *edge connectivity* of G, denoted by $\kappa'(G)$, with at least two vertices is the minimum size of a edge-cut. A graph with at least two vertices is *k-edge-connected* if every edge-cut has at least k edges.

Let $\mathcal{V}_{n,k} = \{G | \kappa(G) \leq k \leq n-1 \text{ and } |G| = n\}$ and $\mathcal{E}_{n,k} = \{G | \kappa'(G) \leq k \leq n-1 \text{ and } |G| = n\}$.

Expansion Lemma. Let G be a k-connected graph, and G' is obtained from G by adding

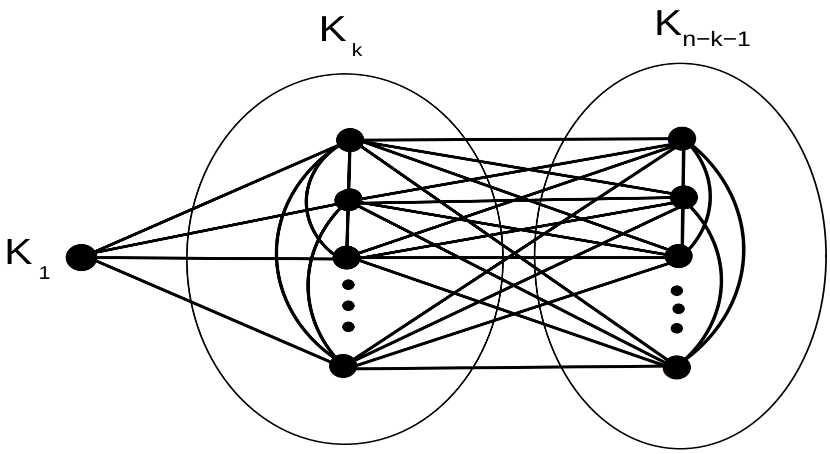

Fig 1: The graph $K\binom{1,k}{n-k-1} = K_1 \diamond K_k \diamond K_{n-k-1}$.

a new vertex u with at least k neighbors in G. Then G' is k-connected.

Two graphs are said to be *disjoint* if they have no vertex in common. Let $G_1, G_2, \cdots, G_l$ be l disjoint graphs, $G_1 \diamond G_2 \diamond \cdots \diamond G_l$ denotes the graph obtained from $G_1 \cup G_2 \cup \cdots \cup G_l$ by joining all the vertices of G_i to those of G_{i+1}, $1 \leq i \leq l-1$.

Let $G\binom{t,k}{n-k-t} = K_t \diamond H_k \diamond K_{n-k-t}$ be a graph with order n, where K_t is the complete graph with order t and H_k is a graph with order k and $k \geq 1, 2 \leq t \leq 2^{-1}(n-k)$.

In particular, if $H_k \cong K_k$, we denote $K\binom{1,k}{n-k-1} = K_1 \diamond K_k \diamond K_{n-k-1}$ be the graph with order n as is shown in Fig. 1, and $K\binom{1,n-1}{0} = K_1 \diamond K_{n-1} = K_n$. By the Expansion Lemma, we obtain that $K\binom{1,k}{n-k-1} \in \mathcal{E}_{n,k} \subseteq \mathcal{V}_{n,k}$.

3 Preliminary lemmas

We begin with several lemmas, which will be helpful to the proofs of our main results.

Lemma 1. *Let G be a simple graph with order n. Then*
(1) $EM_1(G+uv) > EM_1(G)$ for two non-adjacent vertices $u, v \in V(G)$;
(2) $EM_1(G-uv) < EM_1(G)$ for two adjacent vertices $u, v \in V(G)$.

Proof. It follows immediately by the definitions, so omitted here.

Let G be a connected graph with $d_G(u) \geq d_G(v)$ for two non-adjacent vertices u, v. Assume that $v_1, v_2, \cdots, v_s \in N_G(v) \setminus N_G(u)$, where $1 \leq s \leq d_G(v)$. Let $G' = G - \{vv_1, vv_2, \cdots, vv_s\} + \{uv_1, uv_2, \cdots, uv_s\}$. Then we have the following conclusion.

Lemma 2. *Let G and G' be two graphs shown as in Fig. 2. Then $EM_1(G') > EM_1(G)$.*

Proof. For simplicity, we denote $E_1 = \{e|e = ab \in E(G) \text{ and } a, b \neq u, v\}$, $V_1 = N_G(u) \setminus N_G(v)$, $V_2 = N_G(v) \setminus N_G(u)$ and $V_3 = N_G(u) \cap N_G(v)$. Thus we have, see Fig. 2.

$$\begin{aligned} EM_1(G') = & \sum_{ab \in E_1} \Big[d(a) + d(b) - 2\Big]^2 + \sum_{u_i \in V_1} \Big[\Big(d(u) + s\Big) + d(u_i) - 2\Big]^2 \\ & + \sum_{v_i \in V_2} \Big[\Big(d(u) + s\Big) + d(v_i) - 2\Big]^2 + \sum_{w_i \in V_3} \Big[\Big(d(u) + s\Big) + d(w_i) - 2\Big]^2 \\ & + \sum_{w_i \in V_3} \Big[\Big(d(v) - s\Big) + d(w_i) - 2\Big]^2. \end{aligned}$$

By the same reasoning, we have

$$\begin{aligned} EM_1(G) = & \sum_{ab \in E_1} \Big[d(a) + d(b) - 2\Big]^2 + \sum_{u_i \in V_1} \Big[d(u) + d(u_i) - 2\Big]^2 \\ & + \sum_{v_i \in V_2} \Big[d(v) + d(v_i) - 2\Big]^2 + \sum_{w_i \in V_3} \Big[d(u) + d(w_i) - 2\Big]^2 \\ & + \sum_{w_i \in V_3} \Big[d(v) + d(w_i) - 2\Big]^2. \end{aligned}$$

Comparing to the two identities above, we obtain

$$\begin{aligned} EM_1(G') - EM_1(G) = & \sum_{u_i \in V_1} s\Big[2d(u) + 2d(u_i) + s - 4\Big] \\ & + \sum_{v_i \in V_2} \Big[d(u) + s\Big]\Big[d(u) + d(v) + 2d(v_i) + s - 4\Big] \\ & + \sum_{v_i \in V_3} s\Big[2d(u) - 2d(v) + 2s\Big] > 0. \end{aligned}$$

The last inequality follows by $d(u) \geq d(v)$, $d(v) \geq s \geq 1$, $d(u_i) \geq 1$ and $d(v_i) \geq 1$.
This completes the proof. $\square$

Let K_n, P_n and C_n be the complete graph, the path and the cycle with order n, and $K_{p,q}$ be the complete bipartite graph.

Tab. EM_1**-value for some graph families.**

Graph	K_n	$P_n (n > 2)$	C_n	$K_{p,q}$ $(p, q > 2)$
$EM_1 -$ value	$2n(n-1)(n-2)^2$	$4n - 10$	$4n$	$pq(p + q - 2)^2$

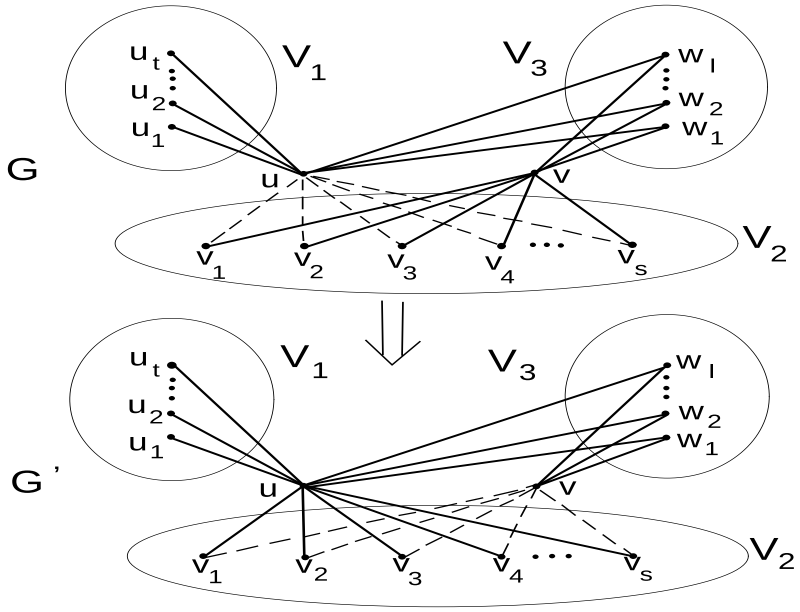

Fig 2: The transformation from graph G to graph G'.
The dotted line illustrates that uv_i is not an edge of G, and analogous illustration for vv_i in G'.

Lemma 3. *(Zhou et al. [3]) Let G be a graph with order n and size $m \geq 1$. Then $EM_1(G) \leq (n-4)M_1(G) + 4M_2(G) - 4m^2 + 4m$, with equality if and only if any two non-adjacent vertices have equal degrees.*

Lemma 4. *(Zhang and Wu [7]) Let G be a graph with order n. Then*
(1) $2^{-1}n(n-1)^2 \leq M_1(G) + M_1(\overline{G}) \leq n(n-1)^2$;
(2) $2^{-3}n(n-1)^3 \leq M_2(G) + M_2(\overline{G}) \leq 2^{-1}n(n-1)^3$.
The upper bounds in (1) and (2) attain on K_n.

Lemma 5. $EM_1\big(G\big(^{t,k}_{n-k-t}\big)\big) < EM_1\big(G\big(^{1,k}_{n-k-1}\big)\big)$ *holds for* $2 \leq t \leq 2^{-1}(n-k)$.

Proof. Let $v_1, v_2, \cdots, v_t$ be the vertices of K_t and $u_1, u_2, \cdots, u_{n-k-t}$ the vertices of K_{n-k-t}. It is obvious that $(t-1)-(n-k-t-1) = 2t-n+k \leq 0$, which implies that $d(u_i) \geq d(v_i)$ holds for all $1 \leq i \leq t$. In view of Lemma 2, we have $EM_1(G'') > EM_1\big(G\big(^{t,k}_{n-k-t}\big)\big)$, where $G'' = G\big(^{t,k}_{n-k-t}\big) - \{v_1v_2, v_1v_3, \cdots, v_1v_t\} + \{u_1v_2, u_1v_3, \cdots, u_1v_t\}$, see Fig. 3. On the other hand, $G\big(^{1,k}_{n-k-1}\big)$ considered to be the graph obtained from G'' by joining u_i and v_h for all $2 \leq i \leq n-k-t$ and $2 \leq h \leq t$. By repeated application of Lemma 1, we have $EM_1(G'') < EM_1\big(G\big(^{1,k}_{n-k-1}\big)\big)$. This completes the proof. □

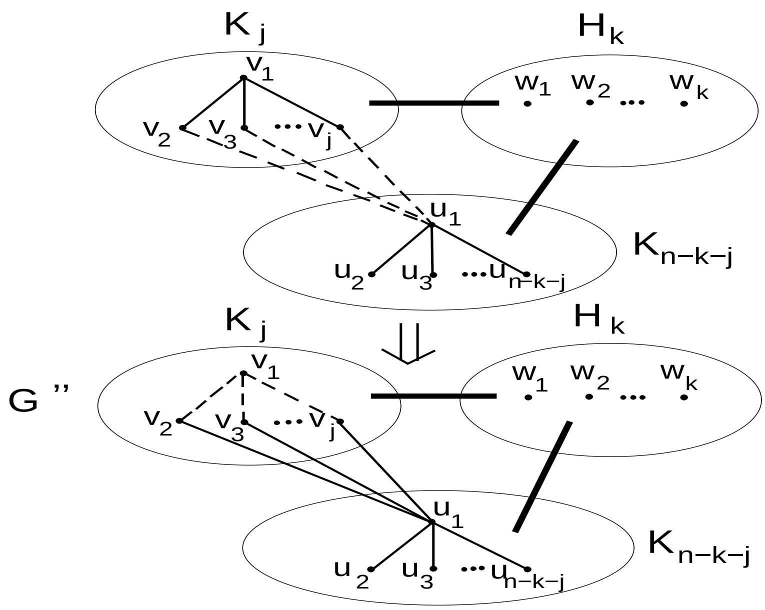

Fig 3: The transformation from graph $G\binom{t,k}{n-k-t}$ to graph G''.
1. The dotted line illustrates that u_1v_i is not an edge of $G\binom{t,k}{n-k-t}$, and analogous illustration for v_1v_i in G''.
2. The bold line between K_t and H_k illustrates the join of them, and analogous illustration for others.

4 The upper and lower bounds of EM_1 index

Theorem 1. *Let G be an arbitrary graph in $\mathcal{V}_{n,k}$. Then*

$$4n-10 \leq EM_1(G) \leq k(k+n-3)^2+4(n-2)^2\binom{k}{2}+4(n-3)^2\binom{n-k-1}{2}+k(n-k-1)(2n-5)^2,$$

the upper bound attains on $K\binom{1,k}{n-k-1}$, and the lower bound attains on P_n.

Proof. (1) We firstly consider the upper bound.

By an elementary calculation, we have
$EM_1\big(K\binom{1,k}{n-k-1}\big) = k(k+n-3)^2+4(n-2)^2\binom{k}{2}+4(n-3)^2\binom{n-k-1}{2}+k(n-k-1)(2n-5)^2$.
We have to prove now that for every $G \in \mathcal{V}_{n,k}$, the inequality $EM_1(G) \leq EM_1\big(K\binom{1,k}{n-k-1}\big)$ holds and with equality if and only if $G \cong K\binom{1,k}{n-k-1}$.

Noting that $K\binom{1,n-1}{0} \cong K_n$ is in the set $\mathcal{V}_{n,k}$. If $k \geq n-1$, the upper bound holds by Lemma 1. If $1 \leq k < n-1$, let G_0 be the graph with order n and maximum EM_1 in $\mathcal{V}_{n,k}$, which implies $EM_1(G) \leq EM_1(G_0)$ holds for all $G \in \mathcal{V}_{n,k}$.

Noting $G_0 \in \mathcal{V}_{n,k}$ is not the complete graph, otherwise $\kappa(G_0) = n-1 \leq k < n-1$, a contradiction to the choice of G_0. Hence there exists a k-vertex cut in G_0, say $S = \{v_1, v_2, \cdots, v_k\}$. Next we have to prove the following several facts:

Fact 1. There are exactly two components in $G_0 - S$.

In fact, suppose that there are at least three components, say $W_1, W_2, \cdots, W_t$ and $t \geq 3$. Let $u \in W_i$ and $v \in W_j$ for any $1 \leq i < j \leq t$. Easily to find that S is also a k-vertex cut of $G_0 + uv$, which means $G_0 + uv \in \mathcal{V}_{n,k}$. By Lemma 1, we obtain $EM_1(G_0 + uv) > EM_1(G_0)$, a contradiction to the choice of G_0. This complete the proof of fact 1.

Without loss of generality, we denote W_1, W_2 be the exactly two components of graph $G_0 - S$.

Fact 2. The graphs induced by $V(W_1) \cup S$ and $V(W_2) \cup S$ are cliques.

In fact, suppose that the graph induced by $V(W_1) \cup S$ is not a clique, hence there exist a pair of non-adjacent vertices $u, v \in V(W_1) \cup S$. Note that $G_0 + uv \in \mathcal{V}_{n,k}$, then we obtain that $EM_1(G_0 + uv) > EM_1(G_0)$ by Lemma 1, again a contradiction, which implies the proof of fact 2.

As desired we know the graphs induced by $V(W_1) \cup S$ and $V(W_2) \cup S$ are cliques, say K_{n_1} and K_{n_2}, respectively.

Fact 3. There is only one clique K_{n_i} such that $|K_{n_i}| = 1$ for $i = 1, 2$.

In fact, suppose that both n_1 and n_2 are larger than 2. Noting $G\binom{1,k}{n-k-1} = K_1 \diamond G_0[S] \diamond K_{n-k-1}$. As is known $G\binom{1,k}{n-k-1} \in \mathcal{V}_{n,k}$. By Lemma 5, we have $EM_1(G_0) < EM_1\big(G\binom{1,k}{n-k-1}\big)$, a contradiction, which implies the proof of fact 3.

This completes the proof of (1).

(2) We now consider the lower bound.

By the table above, we have $EM_1(P_n) = 4n - 10$ for $n > 2$. It remains to prove that for every $G \in \mathcal{V}_{n,k}$, the inequality $EM_1(G) \geq EM_1(P_n)$ holds and with equality if and only if $G \cong P_n$.

Fact 4. P_n takes uniquely the minimum EM_1 on the set of all connected graphs with order n.

In fact, suppose $T_n = \{T | T \text{ is a tree with order } n\}$. Then it is easy to find that the path P_n has the minimum of EM_1 in T_n, respectively. On the other hand, if H is a subgraph of G, then $EM_1(H) \leq EM_1(G)$ holds by Lemma 1. Therefore, the minimum of EM_1 on the set of all connected graphs with order n is the same as the minimum of EM_1 on T_n. This implies that P_n takes the minimum first reformulated Zagreb index EM_1 on the set of all connected graphs with order n.

Now, suppose that $G \in \mathcal{V}_{n,k}$ the graph with EM_1-value as small as possible as described above. Thus among all trees with order n, the path P_n is respectively the unique tree with minimum of EM_1. This implies the proof of fact 4.

As desired we have completed the proof of Theorem 1. □

Theorem 2. *Let G be an arbitrary graph in $\mathcal{E}_{n,k}$. Then*

$$4n-10 \leq EM_1(G) \leq k(k+n-3)^2 + 4(n-2)^2\binom{k}{2} + 4(n-3)^2\binom{n-k-1}{2} + k(n-k-1)(2n-5)^2,$$

the upper bound attains on $K\binom{1,k}{n-k-1}$, and the lower bound attains on P_n.

Proof. Since $K\binom{1,k}{n-k-1} \in \mathcal{E}_{n,k} \subseteq \mathcal{V}_{n,k}$, we immediately complete the proof. □

Theorem 3. *Let G be a graph with order n and size m. Then*

$$EM_1(G) + EM_1(\overline{G}) \leq 2n(n-1)(n-2)^2 + 4n(n-1)m - 8m^2,$$

and the upper bound attains on K_n.

Proof. By applying Lemma 3 to the completement graph $\overline{G}$, one obtains $EM_1(\overline{G}) \leq (n-4)M_1(\overline{G}) + 4M_2(\overline{G}) - 4\overline{m}^2 + 4\overline{m}$, thus $EM_1(G) + EM_1(\overline{G}) \leq (n-4)\big(M_1(G) + M_1(\overline{G})\big) + 4\big(M_2(G) + M_2(\overline{G})\big) - 4(m^2 + \overline{m}^2) + 4(m + \overline{m})$. In view of Lemma 4, $2^{-1}n(n-1)^2 \leq M_1(G) + M_1(\overline{G}) \leq 2^{-1}n(n-1)$, and $2^{-3}n(n-1)^3 \leq M_2(G) + M_2(\overline{G}) \leq 2^{-1}n(n-1)^3$, we complete the proof of the first part by elementary calculations.

Note that the upper bound is best possible. By the table, $EM_1(K_n) + EM_1(\overline{K}_n) = 2n(n-1)(n-2)^2$, the upper bound attains on K_n. □

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