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Research Article

On general reduced second Zagreb index of graphs

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Abstract

Recently, Furtula et al. [B. Furtula, I. Gutman, S. Ediz, On difference of Zagreb indices, Discrete Appl. Math., 2014] introduced a new vertex-degree-based graph invariant "reduced second Zagreb index" in chemical graph theory. Here we generalize the reduced second Zagreb index (call "general reduced second Zagreb index"), denoted by $GRM_\alpha(G)$ and is defined as: $GRM_\alpha(G) = \sum_{uv\in E(G)}(d_G(u)+\alpha)(d_G(v)+\alpha)$, where α is any real number and $d_G(v)$ is the degree of the vertex v of G. Let $\mathcal{G}_n^k$ be the set of connected graphs of order n with k cut edges. In this paper, we study some properties of $GRM_\alpha(G)$ for connected graphs G. Moreover, we obtain the sharp upper bounds on $GRM_\alpha(G)$ in $\mathcal{G}_n^k$ for $\alpha \geq -1/2$ and characterize the extremal graphs.

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1. Introduction

Let $G=(V,E)$ be a connected graph with vertex set $V(G)$ and edge set $E(G)$. Denote by $d_G(u)$, the degree of the vertex u of G. A graph invariant is a number related to a graph which is a structural invariant, in other words, it is a fixed number under graph automorphisms. The oldest and well-known graph invariants are the classical Zagreb indices (M_1 and M_2) of graph G and they are defined as

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

The Zagreb indices M_1 and M_2 were first introduced by Gutman and Trinajstić in 1972, the quantities of the Zagreb indices were found to occur within certain approximate expressions for the total π-electron energy [15]. In 1975, these graph invariants were proposed to be measures of branching of the carbon atom skeleton [14]. For details of the mathematical theory and chemical applications of the Zagreb indices, see [2, 7, 9, 13, 22]. The Zagreb

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indices were independently studied in the mathematical literature under other names [1, 6, 21, 27].

Caporossi and Hansen [3] conjectured that, for all connected graphs G it holds that

$$\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m} \tag{1.1}$$

and the bound is tight for complete graphs. Although this conjecture is disproved for general graphs [16], it was the beginning of a long series of studies in which the validity or non-validity of inequality (1.1) for various classes of graphs, see [16, 18, 20, 25, 26] and the references cited therein.

Recently, much attention is being paid to the comparison of M_1 and M_2. Direct comparisons were obtained on the Zagreb indices for trees [8, 24] and cyclic graphs [4]. The difference of the Zagreb indices of a graph G has been studied in [12, 19].

Furtula, Gutman and Ediz [12] showed that the difference of the Zagreb indices is closely related to the vertex-degree-based graph invariant

$$RM_2(G) = \sum_{uv \in E(G)} (d_G(u) - 1)(d_G(v) - 1)$$

and determined a few basic properties of MR_2. This vertex-degree-based graph invariant RM_2 is called reduced second Zagreb index and it was studied in [12] for trees and in [17] for cyclic graphs with cut edges.

Here we generalize the reduced second Zagreb index (call "general reduced second Zagreb index"), denoted by $GRM_\alpha(G)$ and is defined as:

$$GRM_\alpha(G) = \sum_{uv \in E(G)} (d_G(u) + \alpha)(d_G(v) + \alpha),$$

where α is any real number. It was studied in [1] for general graphs when $\alpha = 1$.

A pendant vertex is a vertex of degree one. An edge of a graph is said to be pendant if one of its end vertices is a pendant vertex. For $v \in V(G)$, $N_G(v)$ denotes the neighbors of v and $N_G[v] = N_G(v) \cup \{v\}$. The maximum vertex degree of G is denoted by $\Delta(G)$. Denote by $\overline{G}$, the complement of graph G. A cut edge in a graph G is an edge whose removal increases the number of connected components of G. For a subset E' of $E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges in E'. For a subset E'' of $E(\overline{G})$, the graph obtained from G by adding a set of edges E'' is denoted by $G + E''$. If $E' = \{e_1\}$ and $E'' = \{e_2\}$, the subgraph $G - E'$ and the super graph $G + E''$ will be written as $G - e_1$ and $G + e_2$ for short, respectively. Denote by $\mathcal{G}_n^k$ the set of connected graphs of order n with k cut edges. Let K_n^k be a graph obtained by joining k pendant vertices to one vertex of the complete graph K_{n-k}. Also denote by $\mathcal{G}_n^{k+}$ the set of connected graphs of order n with at least k cut edges. Then we have $K_n^k \in \mathcal{G}_n^k$, $\mathcal{G}_n^k \subseteq \mathcal{G}_n^{k+}$ and $\mathcal{G}_n^{k+} = \bigcup_{i \geq k} \mathcal{G}_n^i$. Note that a connected graph of order n has at most $n - 1$ cut edges.

The extremal graphs of order n with k cut edges on Zagreb indices were studied in [10, 11]. Namely, it was proved that K_n^k has maximum M_1 or M_2-value in $\mathcal{G}_n^k$. Alternative proof of these results were given in [5].

This paper is organized as follows. In Section 2, some properties of GRM_α are provided. In Section 3, we present the sharp upper bound on GRM_α in $\mathcal{G}_n^k$ for $\alpha > -1/2$ and characterize the extremal graphs. In Section 4, we obtain the sharp upper bound on GRM_α in $\mathcal{G}_n^k$ for $\alpha = -1/2$ and characterize the extremal graphs.

2. Properties of GRM_α

In this section, we provide some properties of GRM_α that will be useful in our study in later sections. From the definitions of M_1 and M_2, we easily get the following identity

$$\begin{aligned} GRM_\alpha(G) &= \sum_{uv\in E(G)} \Big(d_G(u)+\alpha\Big)\Big(d_G(v)+\alpha\Big) \\ &= \sum_{uv\in E(G)} d_G(u)d_G(v) + \alpha \sum_{uv\in E(G)} \Big(d_G(u)+d_G(v)\Big) + \alpha^2\,|E(G)| \\ &= M_2(G) + \alpha M_1(G) + \alpha^2|E(G)| \qquad (2.1) \end{aligned}$$

where α is any real number.

Lemma 2.1. *Let G be a connected graph. Let $uv \in E(G)$ and $N_G(v)\backslash N_G[u] = \{v_1, v_2, \ldots, v_t\} \neq \emptyset$. Consider the graph $G' = G - \{vv_1, vv_2, \ldots, vv_t\} + \{uv_1, uv_2, \ldots, uv_t\}$. Then*
(i) $M_1(G') - M_1(G) = 2t\Big((d_G(u) - d_G(v) + t\Big)$,
(ii) $M_2(G') - M_2(G) \geq t\Big(d_G(u) - d_G(v) + t\Big)$ *when* $d_G(u) \geq d_G(v)$.

Proof. Now we have $d_G(w) = d_{G'}(w)$ for $w \neq u, v$ whereas $d_{G'}(u) = d_G(u) + t$ and $d_{G'}(v) = d_G(v) - t$.

(i) By the definition of M_1, we get

$$\begin{aligned} M_1(G') - M_1(G) &= (d_G(u)+t)^2 + (d_G(v)-t)^2 - d_G(u)^2 - d_G(v)^2 \\ &= 2t\Big((d_G(u) - d_G(v) + t\Big). \end{aligned}$$

(ii) Also, by the definition of M_2, we get

$$\begin{aligned} M_2(G') - M_2(G) &= \sum_{x\in N_G(u)\backslash N_G[v]} \Big(d_G(u)+t\Big)d_G(x) + \sum_{i=1}^{t} \Big(d_G(u)+t\Big)d_G(v_i) \\ &\quad + \sum_{y\in N_G(u)\cap N_G(v)} \Big(d_G(u)+d_G(v)\Big)d_G(y) + \Big(d_G(u)+t\Big)\Big(d_G(v)-t\Big) \\ &\quad - \sum_{x\in N_G(u)\backslash N_G[v]} d_G(u)d_G(x) - \sum_{i=1}^{t} d_G(v)d_G(v_i) \\ &\quad - \sum_{y\in N_G(u)\cap N_G(v)} \Big(d_G(u)+d_G(v)\Big)d_G(y) - d_G(u)d_G(v) \\ &= \sum_{x\in N_G(u)\backslash N_G[v]} t d_G(x) + \sum_{i=1}^{t} \Big(d_G(u) - d_G(v) + t\Big)d_G(v_i) \\ &\qquad - t\,\Big(d_G(u) - d_G(v) + t\Big) \\ &= \sum_{x\in N_G(u)\backslash N_G[v]} t d_G(x) + \sum_{i=1}^{t} \Big(d_G(u) - d_G(v) + t\Big)\Big(d_G(v_i) - 1\Big) \\ &\geq \sum_{x\in N_G(u)\backslash N_G[v]} t\, d_G(x) \geq t\,|N_G(u) \setminus N_G[v]| \qquad (2.2) \end{aligned}$$

since G is connected and $d_G(u) \geq d_G(v)$.

It is easy to see that $N_G(u) \cup \Big(N_G(v) \setminus N_G[u]\Big) = N_G(v) \cup \Big(N_G(u) \setminus N_G[v]\Big)$. Therefore we have

$$|N_G(u)| + |N_G(v) \setminus N_G[u]| = |N_G(v)| + |N_G(u) \setminus N_G[v]|,$$

that is

$$d_G(u) + t = d_G(v) + |N_G(u) \setminus N_G[v]|. \tag{2.3}$$

From (2.2) and (2.3), we get the required result. This completes the proof. □

Lemma 2.2. *Let G be a connected graph. Let $uv \in E(G)$ and $N_G(v) \setminus N_G[u] = \{v_1, v_2, \ldots, v_t\}$. Consider the graph $G' = G - \{vv_1, vv_2, \ldots, vv_t\} + \{uv_1, uv_2, \ldots, uv_t\}$. Then the number of cut edges in G is less than or equal to the number of cut edges in G'.*

Proof. We prove that the number of non-cut edges in G' is less than or equal to the number of non-cut edges in G. Obviously, $|E(G')| = |E(G)|$. Hence it is sufficient to prove that for every non-cut edge in G', there is a corresponding non-cut edge in G.

If uv is a non-cut edge in G', then it is also non-cut edge in G. Conversely, suppose that uv is a cut edge in G. Then $N_G(u) \cap N_G(v) = \emptyset$ and it follows that uv is a pendant edge in G'. But this contradicts the fact that uv is a non-cut edge in G'.

For $1 \leq i \leq t$, if uv_i is a non-cut edge in G', then there is a path Q ($Q \neq uv_i$) from u to v_i in G'. Obviously Q is the subgraph of G'. For the convenience, we denote by $E(Q)$ the edge set of Q. If $uv \in E(Q)$ then $Q - uv$ is a path from v to v_i in G. Otherwise $Q + uv$ is a path from v to v_i in G. Therefore vv_i is a non-cut edge in G for $1 \leq i \leq t$.

Now the proof will be completed by showing that if xy is a non-cut edge in G', which is different from $uv_1, uv_2, \ldots, uv_t$ and uv, then xy must also be a non-cut edge in G. Since xy is a non-cut edge in G', there is a path P ($P \neq xy$) from x to y in G'. Since P is the path, there are at most two edges incident to u in $E(P)$. If $uv_i \notin E(P)$ for each $1 \leq i \leq t$, then P is a path from x to y in G. Thus xy is a non-cut edge in G. Let now $uv_i \in E(P)$ and $uv_s \notin E(P)$ for each $1 \leq s \leq t$ such that $s \neq i$. In this case, if $uv \in E(P)$ then $P - \{uv, uv_i\} + vv_i$ is a path from x to y in G. Otherwise $P - uv_i + \{uv, vv_i\}$ is a path from x to y in G. Finally if $uv_i \in E(P)$, $uv_j \in E(P)$ and $uv_s \notin E(P)$ for each $1 \leq s \leq t$ such that $s \neq i, j$, then $P - \{uv_i, uv_j\} + \{vv_i, vv_j\}$ is a path from x to y in G. This completes the proof. □

Proposition 2.3. *Let G be a graph in $\mathcal{G}_n^{k+}$ and $\alpha > -1/2$. If $GRM_\alpha(G)$ is maximum, then we have $\Delta(G) = n - 1$.*

Proof. By contradiction we will prove this result. For this let u be a maximum degree vertex in G and $d(u) < n - 1$. Since G is connected, there exist the vertices v and v_1 in G such that $uv, vv_1 \in E(G)$ and $uv_1 \notin E(G)$, where v_1 is the vertex at distance 2 from u. Obviously, $v_1 \in N_G(v) \setminus N_G[u]$ and let $N_G(v) \setminus N_G[u] = \{v_1, v_2, \ldots, v_t\}$. Now we consider the graph

$$G' = G - \{vv_1, vv_2, \ldots, vv_t\} + \{uv_1, uv_2, \ldots, uv_t\}.$$

Then, we have $G' \in \mathcal{G}_n^{k+}$ by Lemma 2.2. Obviously, $|E(G')| = |E(G)|$.

Hence by Lemma 2.1 , we get

$$\begin{aligned} GRM_\alpha(G') - GRM_\alpha(G) &= M_2(G') - M_2(G) + \alpha\,(M_1(G') - M_1(G)) \\ &\geq t(1 + 2\alpha)\,(d_G(u) - d_G(v) + t) > 0 \end{aligned}$$

since u is the maximum degree vertex, $t \geq 1$ and $\alpha > -1/2$. Therefore $GRM_\alpha(G') > GRM_\alpha(G)$ for $\alpha > -1/2$, but it contradicts the fact that $GRM_\alpha(G)$ is maximum in $\mathcal{G}_n^{k+}$. Hence $\Delta(G) = n - 1$. □

Corollary 2.4. *Let T be a tree of order n and $\alpha > -1/2$. If $GRM_\alpha(T)$ is maximum, then T is isomorphic to star graph S_n.*

Proposition 2.5. *Let G be a connected graph and $\alpha \geq -1$. Also let $uv \notin E(G)$. Consider the graph $G' = G + uv$. Then*

$$GRM_\alpha(G') > GRM_\alpha(G).$$

Proof. We have $d_G(w) = d_{G'}(w)$ for $w \neq u, v$ whereas $d_{G'}(u) = d_G(u) + 1$ and $d_{G'}(v) = d_G(v) + 1$. Hence by the definition of GRM_α, we get

$$\begin{aligned}
& GRM_\alpha(G') - GRM_\alpha(G) \\
= & \sum_{xy\in E(G')} \Big(d_{G'}(x) + \alpha\Big)\Big(d_{G'}(y) + \alpha\Big) - \sum_{xy\in E(G)} \Big(d_G(x) + \alpha\Big)\Big(d_G(y) + \alpha\Big) \\
= & \sum_{x\in N_G(u)} \Big(d_G(x) + \alpha\Big)\Big(d_G(u) + 1 + \alpha\Big) + \sum_{x\in N_G(v)} \Big(d_G(x) + \alpha\Big)\Big(d_G(v) + 1 + \alpha\Big) \\
& \qquad + \Big(d_G(u) + 1 + \alpha\Big)\Big(d_G(v) + 1 + \alpha\Big) \\
& - \sum_{x\in N_G(u)} \Big(d_G(x) + \alpha\Big)\Big(d_G(u) + \alpha\Big) - \sum_{x\in N_G(v)} \Big(d_G(x) + \alpha\Big)\Big(d_G(v) + \alpha\Big) \\
= & \sum_{x\in N_G(u)} \Big(d_G(x) + \alpha\Big) + \sum_{x\in N_G(v)} \Big(d_G(x) + \alpha\Big) + \Big(d_G(u) + 1 + \alpha\Big)\Big(d_G(v) + 1 + \alpha\Big) \\
> & \ 0
\end{aligned}$$

since $d_G(z) \geq 1$ for all $z \in V(G)$ and $\alpha \geq -1$. This completes the proof. □

An edge uv of a graph G is said to be contracted if it is deleted and its end vertices u and v are identified, the obtained graph is denoted by $G \cdot uv$. Also the identified vertex in $G \cdot uv$ is denoted by one of u and v. A double-star is a tree with exactly two vertices of degree greater than 1. Obviously, a double-star has a unique non-pendant cut edge. Denote by $\mathcal{G}_{n,m}$, the set of connected graphs of order n with m edges.

Proposition 2.6. *Let G be a graph in $\mathcal{G}_{n,m}$. Also let $GRM_\alpha(G)$ be maximum.*
(i) *If $\alpha > -1/2$ then all cut edges of G are pendant.*
(ii) *If $\alpha = -1/2$ and G is different from a double-star, then all cut edges of G are pendant.*

Proof. We prove this result by contradiction. For this let G be a graph with at least one non-pendant cut edge uv in $\mathcal{G}_{n,m}$ and $\alpha \geq -1/2$ such that $GRM_\alpha(G)$ is maximum. Let G' be a graph obtained from $G \cdot uv$ by joining a pendant vertex x to the identified vertex u. Then we have $G' \in \mathcal{G}_{n,m}$. Also, we have $d_{G'}(x) = 1$ and $d_{G'}(\omega) = d_G(\omega)$ for $\omega \neq u$

whereas $d_{G'}(u) = d_G(u) + d_G(v) - 1$. Therefore, we have

$$\begin{aligned} M_2(G') - M_2(G) &= \Big(d_G(u) + d_G(v) - 1\Big)\left(1 + \sum_{u_i \in N_G(u)\setminus\{v\}} d_G(u_i) + \sum_{v_i \in N_G(v)\setminus\{u\}} d_G(v_i)\right) \\ &\quad - d_G(u) \sum_{u_i \in N_G(u)\setminus\{v\}} d_G(u_i) - d_G(v) \sum_{v_i \in N_G(v)\setminus\{u\}} d_G(v_i) - d_G(u) d_G(v) \\ &= \Big(d_G(v) - 1\Big) \sum_{v_i \in N_G(u)\setminus\{v\}} d_G(u_i) + \Big(d_G(u) - 1\Big) \sum_{v_i \in N_G(v)\setminus\{u\}} d_G(v_i) \\ &\quad - \Big(d_G(v) - 1\Big)\Big(d_G(u) - 1\Big) \end{aligned} \tag{2.4}$$

and

$$\begin{aligned} M_1(G') - M_1(G) &= \Big(d_G(u) + d_G(v) - 1\Big)^2 + 1 - d_G(v)^2 - d_G(u)^2 \\ &= 2\Big(d_G(v) - 1\Big)\Big(d_G(u) - 1\Big). \end{aligned} \tag{2.5}$$

Also we have

$$\sum_{v_i \in N_G(u)\setminus\{v\}} d_G(u_i) \geq d_G(u) - 1 \quad \text{and} \quad \sum_{v_i \in N_G(v)\setminus\{u\}} d_G(v_i) \geq d_G(v) - 1. \tag{2.6}$$

From (2.4) and (2.5), using (2.1) and (2.6) we obtain

$$\begin{aligned} & GRM_\alpha(G') - GRM_\alpha(G) = M_2(G') + \alpha M_1(G') - M_2(G) - \alpha M_1(G) \\ &= \Big(d_G(v) - 1\Big) \sum_{v_i \in N_G(u)\setminus\{v\}} d_G(u_i) + \Big(d_G(u) - 1\Big) \sum_{v_i \in N_G(v)\setminus\{u\}} d_G(v_i) \\ &\quad + (2\alpha - 1)\Big(d_G(v) - 1\Big)\Big(d_G(u) - 1\Big) \\ &= \Big(d_G(v) - 1\Big)\Big[\sum_{v_i \in N_G(u)\setminus\{v\}} d_G(u_i) + \Big(\alpha - \frac{1}{2}\Big)\Big(d_G(u) - 1\Big)\Big] \\ &\quad + \Big(d_G(u) - 1\Big)\Big[\sum_{v_i \in N_G(v)\setminus\{u\}} d_G(v_i) + \Big(\alpha - \frac{1}{2}\Big)\Big(d_G(v) - 1\Big)\Big] \\ &\geq (2\alpha + 1)\Big(d_G(v) - 1\Big)\Big(d_G(u) - 1\Big). \end{aligned} \tag{2.7}$$

(i) Since $\alpha > -1/2$ and uv is a non-pendant cut edge in G, from (2.7), we get

$$GRM_\alpha(G') > GRM_\alpha(G). \tag{2.8}$$

It contradicts the assumption that $GRM_\alpha(G)$ is maximum.

(ii) Since $\alpha = -1/2$ and uv is a non-pendant cut edge in G, from (2.7), we get

$$GRM_\alpha(G') \geq GRM_\alpha(G). \tag{2.9}$$

Suppose that equality holds in (2.9). Then from (2.6) and (2.7), we get $d_G(u_i) = 1$ for $u_i \in N_G(u) \setminus \{v\}$ and $d_G(v_i) = 1$ for $v_i \in N_G(v) \setminus \{u\}$. Hence G is isomorphic to a double-star, but it contradicts the assumption. □

The number of cut edges of the considered graph G' in the proof of Proposition 2.6 is equal to the number of cut edges of G. i.e., If $G \in \mathcal{G}_n^k$, then also $G' \in \mathcal{G}_n^k$. Hence we have the following corollary.

Corollary 2.7. *Let G be a graph in $\mathcal{G}_n^k$. Also let $GRM_\alpha(G)$ be maximum.*
(i) *If $\alpha > -1/2$ then all cut edges of G are pendant.*
(ii) *If $\alpha = -1/2$ and G is different from a double-star, then all cut edges of G are pendant.*

3. Maximum GRM_α in $\mathcal{G}_n^k$ for $\alpha > -1/2$

In this section, we give the sharp upper bound on GRM_α in $\mathcal{G}_n^k$ for $\alpha > -1/2$ and characterize the extremal graphs.

Proposition 3.1. *Let G be a graph in $\mathcal{G}_n^{k+}$ and $\alpha > -1/2$. If $GRM_\alpha(G)$ is maximum then G is isomorphic to K_n^k.*

Proof. If $k = n-1$ then G is a tree of order n. Hence we get the required result by Corollary 2.4, because $K_n^k \cong S_n$. Let now $k < n-1$ and G be a graph in $\mathcal{G}_n^{k+} \setminus \{K_n^k\}$ that is not isomorphic to K_n^k such that $GRM_\alpha(G)$ is maximum. Then we prove that

$$GRM_\alpha(G) < GRM_\alpha(K_n^k).$$

Let u be a maximum degree vertex in G. Then $d_G(u) = n-1$, by Proposition 2.3. Hence all cut edges of G are pendant. Let l be the number of cut edges in G. Then $l \geq k$.

First we assume that $l > k$. Let G' be a graph obtained from G by joining one pendant vertex to another non-pendant vertex of G. Then $G' \in \mathcal{G}_n^{k+}$ and

$$GRM_\alpha(G') > GRM_\alpha(G)$$

by Proposition 2.5. It contradicts the fact that $GRM_\alpha(G)$ is maximum in $\mathcal{G}_n^{k+}$.

Next we assume that $l = k$. Then since G is not isomorphic to K_n^k, there exist two non-adjacent vertices of degrees greater than one in the graph G. We join these two non-adjacent vertices and denote by G' the obtained graph. Then $G' \in \mathcal{G}_n^{k+}$ and

$$GRM_\alpha(G') > GRM_\alpha(G)$$

by Proposition 2.5. If G' is isomorphic to K_n^k then we are done. Otherwise, a contradiction. This completes the proof. $\square$

Theorem 3.2. *Let G be a graph in $\mathcal{G}_n^k$ and $\alpha > -1/2$. Then*

$$\begin{aligned} GRM_\alpha(G) \;\leq\; & \frac{1}{2}(n-k-1)(n-k-1+\alpha)\Big[(n-k)(n-k-1+\alpha)+2k\Big] \\ & +k(n-1+\alpha)(1+\alpha) \end{aligned}$$

with equality holding if and only if G is isomorphic to K_n^k.

Proof. Since $K_n^k \in \mathcal{G}_n^k$ and $\mathcal{G}_n^k \subseteq \mathcal{G}_n^{k+}$, by Proposition 3.1, we have

$$GRM_\alpha(G) < GRM_\alpha(K_n^k)$$

for all $G \in \mathcal{G}_n^k$ with $G \ncong K_n^k$ and for $\alpha > -1/2$. By the definition of GRM_α we get

$$\begin{aligned} & GRM_\alpha(K_n^k) \\ = \;& (n-1+\alpha)\Big[(1+\alpha)k+(n-k-1+\alpha)(n-k-1)\Big]+\binom{n-k-1}{2}(n-k-1+\alpha)^2 \\ = \;& (n-1+\alpha)(1+\alpha)k+(n-k-1)(n-k-1+\alpha)\Big[n-1+\alpha+\frac{(n-k-2)(n-k-1+\alpha)}{2}\Big] \\ = \;& (n-1+\alpha)(1+\alpha)k+\frac{1}{2}(n-k-1)(n-k-1+\alpha)\Big[(n-k)(n-k-1+\alpha)+2k\Big]. \end{aligned}$$

From the above, we get the required result. □

Corollary 3.3. [5,10,11] *Let G be a graph in $\mathcal{G}_n^k$. Then*

$$M_2(G) \leq \frac{1}{2}(n-k-1)^3(n-k-2) + [(n-k-1)^2 + k](n-1)$$

with equality holding if and only if G is isomorphic to K_n^k.

Proof. Taking $\alpha = 0$ in Theorem 3.2, we get the required result. □

4. Maximum $GRM_{-1/2}$ in $\mathcal{G}_n^k$

In this section, we give the sharp upper bound on $GRM_{-1/2}$ in $\mathcal{G}_n^k$ and characterize the extremal graphs.

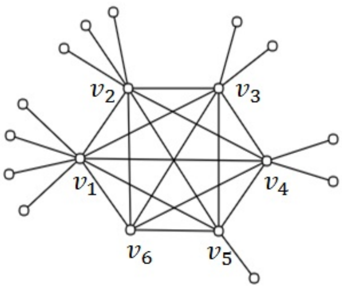

Fig. 1. The graph $G(4,3,2,2,1,0)$ in $\mathcal{G}(18,6) \subseteq \mathcal{G}_{18}^{12}$.

Let N be a positive integer, $N \geq 1$. Denote by K_N, a complete graph of order N, and let $v_1, v_2, \ldots, v_N$ be its vertices. For $i = 1, 2, \ldots, N$, let r_i be non-negative integers, labeled so that $r_1 \geq r_2 \geq \cdots \geq r_N \geq 0$. Construct the graph $G(r_1, r_2, \ldots, r_N)$ by attaching r_i pendent vertices to the vertex v_i of K_N. The graph $G(r_1, r_2, \ldots, r_N)$ has thus $n = N + \sum_{i=1}^{N} r_i$ vertices. For given values $n \geq N \geq 1$, the set of all graphs $G(r_1, r_2, \ldots, r_N)$ constructed in the above described manner is denoted by $\mathcal{G}(n, N)$ (see Fig. 1). If $N = 1$ then $\mathcal{G}(n, 1) = \{S_n\}$ and if $N = 2$ then $\mathcal{G}(n, 2)$ is the set of all double-stars of order n.

We now calculate the value on $GRM_{-1/2}(G)$ for the graphs G in $\mathcal{G}(n, N)$.

Lemma 4.1. *Let G be a graph in $\mathcal{G}(n, n-k)$. Then*

$$GRM_{-1/2}(G) \quad = \quad \frac{1}{2}\left(n - \frac{3}{2}\right)k + \frac{1}{2}\left(n-k-\frac{3}{2}\right)(n-k-1)\left[(n-k)^2 + \frac{7}{2}k - \frac{3}{2}n\right].$$

Proof. Since $G \in \mathcal{G}(n, n-k)$, there exist nonnegative integers $r_1, r_2, \ldots, r_{n-k}$, labeled so that $r_1 \geq r_2 \geq \cdots \geq r_{n-k} \geq 0$ with $r_1 + r_2 + \cdots + r_{n-k} = k$ and $G \cong G(r_1, r_2, \ldots, r_{n-k})$. Let $v_1, v_2, \ldots, v_{n-k}$ be vertices of the graph $G(r_1, r_2, \ldots, r_{n-k})$ whose degrees greater than one. Then $d_G(v_i) = r_i + n - k - 1$ for $i = 1, 2, \ldots, n-k$,

$$\sum_{i=1}^{n-k} r_i^2 + 2 \sum_{1 \leq i < j \leq n-k} r_i r_j = k^2 \quad \text{and} \quad \sum_{1 \leq i < j \leq n-k} (r_i + r_j) = (n-k-1)k.$$

Therefore, by using the above we get

$$
\begin{aligned}
& GRM_{-1/2}(G) \\
= \; & \sum_{i=1}^{n-k}\Big(r_i+n-k-1-\frac{1}{2}\Big)\Big(1-\frac{1}{2}\Big)r_i \\
& + \sum_{1\le i<j\le n-k}\Big(r_i+n-k-1-\frac{1}{2}\Big)\Big(r_j+n-k-1-\frac{1}{2}\Big) \\
= \; & \frac{1}{2}\Big(n-k-\frac{3}{2}\Big)\sum_{i=1}^{n-k} r_i+\frac{1}{2}\sum_{i=1}^{n-k} r_i^2+\sum_{1\le i<j\le n-k} r_ir_j+\Big(n-k-\frac{3}{2}\Big)\sum_{1\le i<j\le n-k}(r_i+r_j) \\
& \qquad +\Big(n-k-\frac{3}{2}\Big)^2\binom{n-k}{2} \\
= \; & \frac{1}{2}\Big(n-k-\frac{3}{2}\Big)k+\frac{1}{2}k^2+\Big(n-k-\frac{3}{2}\Big)(n-k-1)k+\Big(n-k-\frac{3}{2}\Big)^2\binom{n-k}{2} \\
= \; & \frac{1}{2}\Big(n-\frac{3}{2}\Big)k+\frac{1}{2}\Big(n-k-\frac{3}{2}\Big)(n-k-1)\Big[(n-k)^2+\frac{7}{2}k-\frac{3}{2}n\Big].
\end{aligned}
$$

□

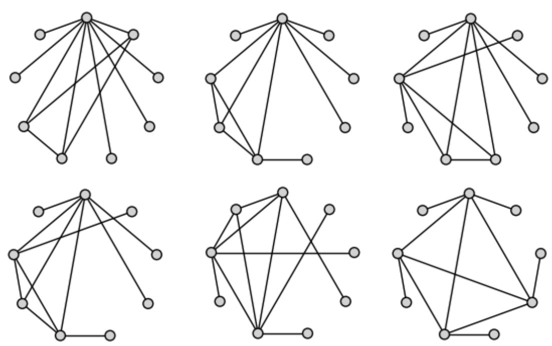

Fig. 2. All graphs G in $\mathcal{G}(9,4) \subseteq \mathcal{G}_9^5$ with maximum value $GRM_{-1/2}(G) = 93.75$.

If G is a tree of order n then $k = n-1$ and

$$GRM_{-1/2}(G) = \frac{(2n-3)(n-1)}{4} \tag{4.1}$$

for $G \in \{S_n\} \cup \mathcal{G}(n,2)$, by the above Lemma 4.1. From the definition of $\mathcal{G}(n,N)$, we have $\{S_n\} \cup \mathcal{G}(n,2) \subseteq \mathcal{G}_n^{n-1}$ and $\mathcal{G}(n,N) \subseteq \mathcal{G}_n^{n-N}$ for $N \geq 3$. There is no connected graph of order n with $n-2$ cut edges. Therefore, we further denote $\mathcal{G}(n,1) = \{S_n\} \cup \mathcal{G}(n,2)$.

Proposition 4.2. *Let G be a graph in $\mathcal{G}_n^k$. If $GRM_{-1/2}(G)$ is maximum, then $G \in \mathcal{G}(n, n-k)$.*

Proof. First, let $k = n-1$. If G is different from a double-star then all cut edges of G are pendant, by Corollary 2.7 (ii). Hence G is isomorphic to star S_n and $S_n \in \mathcal{G}(n,1)$. If G is isomorphic to a double-star, then $G \in \mathcal{G}(n,1)$ and $GRM_{-1/2}(G)$ is also maximum in $\mathcal{G}_n^{n-1}$, because

$$GRM_{-1/2}(G) = GRM_{-1/2}(S_n)$$

from (4.1).

Let now $k < n-1$. Then G is different from a tree. Hence by Corollary 2.7 (ii), all k cut edges of G are pendant. If $G \notin \mathcal{G}(n, n-k)$ then there exist two non-adjacent vertices of degrees greater than one in the graph G. We join these two non-adjacent vertices and denote by G' the obtained graph. Then $G' \in \mathcal{G}_n^k$ and $GRM_{-1/2}(G') > GRM_{-1/2}(G)$ by Lemma 2.3. But it contradicts the fact that $GRM_{-1/2}(G)$ is maximum in $\mathcal{G}_n^k$. □

Theorem 4.3. *Let G be a graph in $\mathcal{G}_n^k$. Then*

$$GRM_{-1/2}(G) \leq \frac{1}{2}\left(n-\frac{3}{2}\right)k+\frac{1}{2}\left(n-k-\frac{3}{2}\right)(n-k-1)\left[(n-k)^2+\frac{7}{2}k-\frac{3}{2}n\right]$$

with equality holding if and only if $G \in \mathcal{G}(n, n-k)$.

Proof. If $G \in \mathcal{G}(n, n-k)$ then the equality holds in the above inequality for G, by Lemma 4.1. Otherwise the inequality is strict, by Proposition 4.2. □

Example 4.4. By SageMath [23], we characterize all graphs in $\mathcal{G}_9^5$ that achieve the bound in Theorem 4.3 (see, Fig. 2).

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