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On General Reduced Second Zagreb Index of Graphs

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Abstract: Graph-based molecular structure descriptors (often called "topological indices") are useful for modeling the physical and chemical properties of molecules, designing pharmacologically active compounds, detecting environmentally hazardous substances, etc. The graph invariant GRM_α, known under the name general reduced second Zagreb index, is defined as $GRM_\alpha(\Gamma) = \sum_{uv \in E(\Gamma)}(d_\Gamma(u)+\alpha)(d_\Gamma(v)+\alpha)$, where $d_\Gamma(v)$ is the degree of the vertex v of the graph Γ and α is any real number. In this paper, among all trees of order n, and all unicyclic graphs of order n with girth g, we characterize the extremal graphs with respect to GRM_α ($\alpha \geq -\frac{1}{2}$). Using the extremal unicyclic graphs, we obtain a lower bound on $GRM_\alpha(\Gamma)$ of graphs in terms of order n with k cut edges, and completely determine the corresponding extremal graphs. Moreover, we obtain several upper bounds on GRM_α of different classes of graphs in terms of order n, size m, independence number γ, chromatic number k, etc. In particular, we present an upper bound on GRM_α of connected triangle-free graph of order $n > 2$, $m > 0$ edges with $\alpha > -1.5$, and characterize the extremal graphs. Finally, we prove that the Turán graph $T_n(k)$ gives the maximum GRM_α ($\alpha \geq -1$) among all graphs of order n with chromatic number k.

Keywords: Zagreb indices; girth; clique number; chromatic number; Turán graph

MSC: 05C07; 05C35

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1. Introduction

Let $\Gamma = (V, E)$ be a simple graph with vertex set $V = V(\Gamma)$ and edge set $E = E(\Gamma)$, where $|V(\Gamma)| = n$ and $|E(\Gamma)| = m$. The degree of the vertex u of Γ, denoted $d_\Gamma(u)$, is the number of vertices adjacent to the vertex u. For $v \in V(\Gamma)$, $N_\Gamma(v)$ denotes the set of vertices adjacent to v, that is, $|N_\Gamma(v)| = d_\Gamma(v)$. Let $\Delta(\Gamma)$ be the maximum degree of graph Γ. As usual, $\chi(\Gamma)$, $\omega(\Gamma)$, $\gamma(\Gamma)$, and g denote, respectively, the chromatic number, the clique number, the independence number, and the girth. Let K_n be the complete graph of order n, and also let $K_{n_1,n_2,\ldots,n_k}$ ($n = n_1 + n_2 + \cdots + n_k$) be a complete k-partite graph of order n. The Turán graph $T_n(k)$ is the complete k-partite graph on n vertices whose partite sets differ in size by at most 1. An edge is a cut edge if, and only if, it is not contained in any cycle. For $F \subseteq E(\Gamma)$, $\Gamma - F$ denotes the graph obtained from Γ by removing the edges in F. Similarly, the graph obtained from Γ by adding a set of edges F is denoted by $\Gamma + F$. For $F = \{e\}$, we write $\Gamma - e$ and $\Gamma + e$. We skip the definitions of other standard graph-theoretical notions, these can be found in [1–3] and other textbooks.

The most famous and studied degree-based topological indices of a graph are the first Zagreb index M_1 and second Zagreb index M_2 of a graph Γ, are defined as

$$M_1(\Gamma) = \sum_{u \in V(\Gamma)} d_\Gamma(u)^2 \quad \text{and} \quad M_2(\Gamma) = \sum_{uv \in E(\Gamma)} d_\Gamma(u) d_\Gamma(v), \tag{1}$$

respectively. The quantities $M_1(\Gamma)$ and $M_2(\Gamma)$ were found to occur within certain approximate expressions for the total π-electron energy [4]. For more informations on the mathematical theory and chemical applications of the Zagreb indices, see [5–44] and the references cited therein. The Zagreb indices has been studied independently in the mathematical literature under other names in [45–50].

Li et al. [51] studied on the extremal cacti of given parameters with respect to the difference of Zagreb indices. Furtula et al. [52] presented some results on $M_2(\Gamma) - M_1(\Gamma)$ and then showed that $M_2(\Gamma) - M_1(\Gamma)$ is closely related to the reduced second Zagreb index, which is defined as

$$RM_2(\Gamma) = \sum_{uv \in E(\Gamma)} (d_\Gamma(u) - 1)(d_\Gamma(v) - 1).$$

The Wiener polarity index, denoted by $W_p(\Gamma)$, is defined as the number of unordered pairs of vertices that are at distance 3 in Γ. When the graph Γ is isomorphic to a tree, we have $RM_2(\Gamma) = W_p(\Gamma)$ and it was examined in the recent papers [52–54]. An and Xiong [55] gave some bounds on $RM_2(\Gamma)$ in terms of vertex connectivity, independence number, and matching number, and also characterized the extremal graphs. In [56], the authors obtained the extremal graphs for $RM_2(\Gamma)$ in the class of cyclic graphs of order n with k cut edges. In [57], some upper bounds of RM_2 were estimated and the extremal graphs with respect to RM_2 among all unicyclic graphs of order n with girth g were characterized.

In [58], Horoldagva et. al studied a generalization of both the reduced second Zagreb index and the second Zagreb index, which is defined as

$$GRM_\alpha(\Gamma) = \sum_{uv \in E(\Gamma)} (d_\Gamma(u) + \alpha)(d_\Gamma(v) + \alpha) = M_2(\Gamma) + \alpha M_1(\Gamma) + \alpha^2 |E(\Gamma)|. \quad (2)$$

and named it general reduced second Zagreb index, where α is any real number. They characterized some properties of GRM_α and the extremal graphs of order n with k cut edges with maximum GRM_α when $\alpha \geq -\frac{1}{2}$.

The structure of the paper is as follows. We give a list of propositions and preliminaries in Section 2. Among all trees of order n, and all unicyclic graphs of order n with girth g, we characterize the extremal graphs with respect to GRM_α ($\alpha \geq -\frac{1}{2}$) in Section 3. Using the extremal unicyclic graphs, we determine the lower bound for the general reduced second Zagreb index of graphs of order n with k cut edges and completely determine the corresponding extremal graphs in Section 4. In Section 5, we obtain several upper bounds on GRM_α of different class of graphs in terms of order n, size m, independence number γ, chromatic number k, etc. In particular, we present an upper bound on GRM_α of connected triangle-free graph of order $n > 2$, $m > 0$ edges with $\alpha > -1.5$, and characterize the extremal graphs. Finally, we prove that the Turán graph $T_n(k)$ gives the maximum GRM_α ($\alpha \geq -1$) among all graphs of order n with chromatic number k.

2. Preliminaries

Here, we list some previously known results and their direct consequences, which are used to prove our main results. The following propositions were proved in [58].

Proposition 1 ([58])**.** *Let Γ be a connected graph, and $\alpha \geq -1$. Additionally, let $xy \notin E(\Gamma)$. Consider the graph $\Gamma' = \Gamma + xy$. Then*

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

Denote by $\mathcal{G}_{n,m}$ the set of connected graphs of order n with m edges.

Proposition 2 ([58])**.** *Let Γ be a graph in $\mathcal{G}_{n,m}$. Additionally, let $GRM_\alpha(\Gamma)$ be maximum.*
(i) If $\alpha > -1/2$ then all cut edges of Γ are pendant.
(ii) If $\alpha = -1/2$, and Γ is different from a double-star, then all cut edges of Γ are pendant.

In [59], the upper bounds in terms of order and size for the Zagreb indices of K_{r+1}-free graphs were given. Two of these bounds are stated as the next proposition.

Proposition 3 ([57,59]). *Let Γ be a K_{r+1}-free graph with n vertices $(2 \leq r \leq n-1)$ and $m > 0$ edges. Then*

$$M_1(\Gamma) \leq \frac{2r-2}{r} nm \quad \text{and} \quad M_2(\Gamma) \leq \frac{2}{r} m^2 + \frac{r-2}{2r} n M_1(\Gamma).$$

Moreover, both equalities hold if, and only if, Γ is isomorphic to a regular complete r-partite graph for $r \geq 3$, and a complete bipartite graph for $r = 2$.

In [57,60], it is proved that the Turán graph $T_{n,\chi}$ gives the maximum Zagreb indices and reduced second Zagreb index among all graphs of order n with chromatic number χ. From the proof of these results, we can formulate the following proposition. We denote $\Delta M(\Gamma) = M_2(\Gamma) - M_1(\Gamma)$.

Proposition 4. *Let $\Gamma \cong K_{n_1,n_2,\ldots,n_k}$ such that $n_q - n_p \geq 2$ for some integers p, q with $1 \leq p < q \leq k$. Additionally, let $\Gamma' \cong K_{n_1,\ldots,n_{p-1},n_p+1,n_{p+1}\ldots,n_{q-1},n_q-1,n_{q+1}\ldots,n_k}$. Then we have*

$$M_1(\Gamma') - M_1(\Gamma) > 0 \quad \text{and} \quad \Delta M(\Gamma') - \Delta M(\Gamma) > 0.$$

3. Maximum and Minimum GRM_α in Trees and Unicyclic Graphs

A star, denoted S_n is a tree with only one vertex of degree greater than one. A double-star is a tree with diameter 3. Let $T_{a,b}$ be a double-star, where degrees of non-pendant vertices are a and b. Then we have

$$GRM_\alpha(S_n) = (n-1+\alpha)(1+\alpha)(n-1)$$

and

$$\begin{aligned} GRM_\alpha(T_{a,b}) &= (a+\alpha)(1+\alpha)(a-1) + (b+\alpha)(1+\alpha)(b-1) + (a+\alpha)(b+\alpha) \\ &= (1+\alpha)(a^2+b^2) + ab + (\alpha^2 - 1 + \alpha)(a+b) - \alpha^2 - 2\alpha. \end{aligned}$$

If $\alpha = -\frac{1}{2}$ then we can easily get

$$GRM_{-1/2}(T_{a,b}) = \frac{1}{2}(a+b)^2 - \frac{5}{4}(a+b) + \frac{3}{4} = GRM_{-1/2}(S_{a+b}).$$

Since each edge in a tree is cut edge, one can easily obtain the following theorem using the above result with Proposition 2.

Theorem 1. *Let T be a tree of order n and $\alpha \geq -1/2$. Then*

$$GRM_\alpha(T) \leq (n-1+\alpha)(1+\alpha)(n-1)$$

with equality if, and only if,
(i) T is isomorphic to star graph S_n if $\alpha > -1/2$,
(ii) T is isomorphic to star graph or double-star if $\alpha = -1/2$.

Before determining the minimum value of GRM_α for trees of order n, we introduce the following transformation:

Transformation D**:** Let Γ be a connected graph of order greater than one with $v \in V(\Gamma)$. Let Γ_1 be the graph obtained from Γ by attaching two new paths $P: v(=v_0)v_1v_2\cdots v_p$ and $Q: v(=v_0)u_1u_2\cdots u_q$ of length p and q, respectively, at v, where $v_1, v_2, \ldots, v_p$ and $u_1, u_2, \ldots, u_q$ are distinct new vertices. A graph Γ_2 is obtained from Γ_1 by deleting vu_1 and adding u_1v_p, as shown in Figure 1.

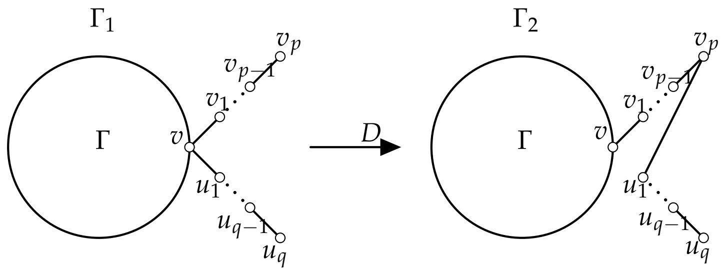

Figure 1. Transformation D.

Now, we prove a lemma that shows that the general reduced second Zagreb index is decreasing by Transformation D when $\alpha \geq -\frac{1}{2}$ and it will play an important role in the proof of the next result.

Lemma 1. *Let Γ_1 and Γ_2 be the graphs in Figure 1.*
(i) Let $\alpha > -\frac{1}{2}$. Then $GRM_\alpha(\Gamma_1) > GRM_\alpha(\Gamma_2)$.
(ii) Let $\alpha = -\frac{1}{2}$ and $p = q = 1$. Then $GRM_\alpha(\Gamma_1) > GRM_\alpha(\Gamma_2)$ if $\sum_{x\in N_\Gamma(v)} d_\Gamma(x) > d_\Gamma(v)$.
(iii) Let $\alpha = -\frac{1}{2}$ and $p + q > 2$. Then $GRM_\alpha(\Gamma_1) > GRM_\alpha(\Gamma_2)$.

Proof. From (1), we obtain

$$M_1(\Gamma_1) - M_1(\Gamma_2) = (d_\Gamma(v) + 2)^2 + 1 - (d_\Gamma(v) + 1)^2 - 4 = 2d_\Gamma(v) > 0.$$

Now,

$$\begin{aligned} M_2(\Gamma_1) - M_2(\Gamma_2) &= (d_\Gamma(v) + 2)\Big(\sum_{x\in N_\Gamma(v)} d_\Gamma(x) + d_{\Gamma_1}(v_1) + d_{\Gamma_1}(u_1)\Big) \\ &\quad + d_{\Gamma_1}(v_{p-1})d_{\Gamma_1}(v_p) - (d_\Gamma(v) + 1)\Big(\sum_{x\in N_\Gamma(v)} d_\Gamma(x) + d_{\Gamma_2}(v_1)\Big) \\ &\quad - d_{\Gamma_2}(v_{p-1})d_{\Gamma_2}(v_p) - d_{\Gamma_2}(v_p)d_{\Gamma_2}(u_1) \\ &= \begin{cases} \sum_{x\in N_\Gamma(v)} d_\Gamma(x) & \text{if } p = q = 1, \\ \sum_{x\in N_\Gamma(v)} d_\Gamma(x) + d_\Gamma(v) & \text{if } q = 1 \text{ and } p > 1, \\ \sum_{x\in N_\Gamma(v)} d_\Gamma(x) + d_\Gamma(v) & \text{if } q > 1 \text{ and } p = 1, \\ \sum_{x\in N_\Gamma(v)} d_\Gamma(x) + 2d_\Gamma(v) & \text{if } q > 1 \text{ and } p > 1. \end{cases} \end{aligned}$$

Since $\mid E(\Gamma_1) \mid = \mid E(\Gamma_2) \mid$ and the Equation (2), we obtain

$$\begin{aligned} GRM_\alpha(\Gamma_1) - GRM_\alpha(\Gamma_2) &= M_2(\Gamma_1) - M_2(\Gamma_2) + \alpha\big(M_1(\Gamma_1) - M_1(\Gamma_2)\big) \\ &= \begin{cases} \sum_{x\in N_\Gamma(v)} d_\Gamma(x) + 2\alpha d_\Gamma(v) & \text{if } p = q = 1, \\ \sum_{x\in N_\Gamma(v)} d_\Gamma(x) + (1 + 2\alpha)d_\Gamma(v) & \text{if } q = 1 \text{ and } p > 1, \\ \sum_{x\in N_\Gamma(v)} d_\Gamma(x) + (1 + 2\alpha)d_\Gamma(v) & \text{if } q > 1 \text{ and } p = 1, \\ \sum_{x\in N_\Gamma(v)} d_\Gamma(x) + (2 + 2\alpha)d_\Gamma(v) & \text{if } q > 1 \text{ and } p > 1. \end{cases} \end{aligned}$$

If $\alpha > -\frac{1}{2}$, then clearly $GRM_\alpha(\Gamma_1) - GRM_\alpha(\Gamma_2) > 0$. Let $\alpha = -\frac{1}{2}$. When $p = q = 1$, $\sum\limits_{x \in N_\Gamma(v)} d_\Gamma(x) + 2\alpha d_\Gamma(v) = \sum\limits_{x \in N_\Gamma(v)} d_\Gamma(x) - d_\Gamma(v) > 0$, that is, $GRM_\alpha(\Gamma_1) - GRM_\alpha(\Gamma_2) > 0$. Otherwise, clearly $GRM_\alpha(\Gamma_1) - GRM_\alpha(\Gamma_2) > 0$. The proof is finished. □

Repeating the Transformation D, any tree can be changed into a path. Thus, we can obtain the next theorem.

Theorem 2. *Let T be a tree of order n and $\alpha \geq -1/2$. Then*

$$GRM_\alpha(T) \geq (\alpha + 2)(n + 2\alpha - 1)$$

with equality if, and only if, $T \cong \begin{cases} P_4 \text{ or } S_4 & \text{if } n = 4 \text{ and } \alpha = -\frac{1}{2}, \\ P_n & \text{otherwise.} \end{cases}$.

We now determine the extremal unicyclic graphs with respect to general reduced second Zagreb index. First, we give a sharp upper bound of GMR_α of graphs from the class of connected unicyclic graphs of order n with girth g, denoted by $\mathcal{U}_{n,g}$ when $\alpha \geq -\frac{1}{2}$. Let $S(n_1, n_2, \ldots, n_g)$ be a unicyclic graph of order n with girth g and $n - g$ pendant vertices (see, Figure 2), where n_i is the number of pendant vertices adjacent to i-th vertex of the cycle (the vertices in the cycle are numbered clockwise). Then, clearly $C_n \cong S(0, 0, \ldots, 0)$ and $\sum\limits_{i=1}^{g} n_i = n - g$. We denote by $\mathcal{S}_{n,g}$ (n and g are integers with $4 \leq g \leq n$) the class of all unicyclic graphs $S(n_1, n_2, \ldots, n_g)$ ($g \geq 5$), such that $|n_1 + n_3 - n_2| \leq 1$ and $n_4 = n_5 = \cdots = n_g = 0$, and $S(n_1, n_2, n_3, n_4)$, such that $|n_1 + n_3 - (n_2 + n_4)| \leq 1$.

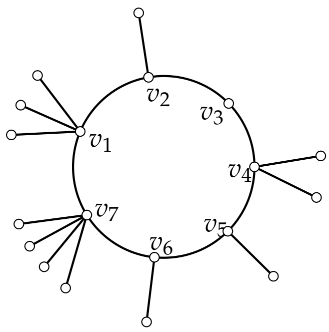

Figure 2. The graph $S(3, 1, 0, 2, 1, 1, 4)$.

Lemma 2. *Let $g \geq 3$ be an integer, α be a real number and $\Gamma \cong S(n_1, n_2, \underbrace{0, \ldots, 0}_{g-2})$, where n_1, n_2 are non-negative integers, such that $n_1 + n_2 = n - g$. Then*

$$GRM_\alpha(\Gamma) = (1 + \alpha)(n - g)^2 + (\alpha + 2)(\alpha + 3)n - (\alpha + 2)g - (2\alpha + 1)n_1 n_2.$$

Proof. By the definition of GRM_α, we have

$$\begin{aligned} GRM_\alpha(\Gamma) &= (n_1 + 2 + \alpha)(n_2 + 2 + \alpha) + (n_1 + 2 + \alpha)(1 + \alpha)n_1 + (n_2 + 2 + \alpha)(1 + \alpha)n_2 \\ &\quad + (g - 3)(2 + \alpha)^2 + (2 + \alpha)(n_1 + 2 + \alpha) + (2 + \alpha)(n_2 + 2 + \alpha) \\ &= n_1 n_2 + (2 + \alpha)(n - g) + (2 + \alpha)^2 + (1 + \alpha)\Big(n_1^2 + n_2^2 + (2 + \alpha)(n - g)\Big) \\ &\quad + (2 + \alpha)^2(g - 3) + (2 + \alpha)(n - g + 4 + 2\alpha) \\ &= (1 + \alpha)(n - g)^2 + (3 + \alpha)(2 + \alpha)n - (\alpha + 2)g - (2\alpha + 1)n_1 n_2. \end{aligned}$$

This completes the proof of the lemma. □

Note that for the graph $\Gamma \cong S(n_1, n_2, \underbrace{0, \ldots, 0}_{g-2})$, $GRM_{-1/2}(\Gamma)$ depends only on n and g. We denote by $\mathcal{H}$ the set of all unicyclic graphs $S(n_1, n_2, \underbrace{0, \ldots, 0}_{g-2})$, such that $\lceil \frac{n-g}{2} \rceil \leq n_1 \leq n - g$ and $n_1 + n_2 = n - g$, where n and g are integers with $3 \leq g \leq n$. Denote by $\mathcal{G}(n, N)$ the set of graphs of order n with clique number $n - N$ and all the remaining N vertices are pendant.

Theorem 3. *Let $\alpha \geq -\frac{1}{2}$, $g \geq 3$ and $\Gamma \in \mathcal{U}_{n,g}$. Then*

$$GRM_\alpha(\Gamma) \leq (1 + \alpha)(n - g)^2 + (\alpha + 2)(\alpha + 3)n - (\alpha + 2)g \tag{3}$$

with equality if, and only if,
(i) $\Gamma \cong S(n - g, \underbrace{0, \ldots, 0}_{g-1})$ when $\alpha > -\frac{1}{2}$,
(ii) $\Gamma \in \mathcal{H}$ when $\alpha = -\frac{1}{2}$ and $g \geq 4$,
(iii) $\Gamma \in \mathcal{G}(n, n - 3)$ when $\alpha = -\frac{1}{2}$ and $g = 3$.

Proof. Let Γ_0 be a unicyclic graph of order n with girth g and maximum GRM_α-value. Then we have

$$GRM_\alpha(\Gamma) \leq GRM_\alpha(\Gamma_0). \tag{4}$$

By Proposition 2, all cut edges of Γ_0 are pendant. Hence, there exist non-negative integers $n_1, n_2, \ldots, n_g$ such that $\sum\limits_{i=1}^{g} n_i = n - g$ and $\Gamma_0 \cong S(n_1, n_2, \ldots, n_g)$. Let $v_1, v_2, \ldots, v_g$ be the vertices of the graph $S(n_1, n_2, \ldots, n_g)$ whose degrees are greater than one. Then we have $d_{\Gamma_0}(v_i) = n_i + 2$ for $i = 1, 2, \ldots, g$. From (2), we obtain

$$\begin{aligned}
GRM_\alpha(\Gamma_0) &= \sum_{i=1}^{g}(n_i + 2 + \alpha)(n_{i+1} + 2 + \alpha) + \sum_{i=1}^{g}(n_i + 2 + \alpha)(1 + \alpha)n_i \\
&= \sum_{i=1}^{g} n_i n_{i+1} + (\alpha + 2)\sum_{i=1}^{g}(n_i + n_{i+1}) + (\alpha + 2)^2 g \\
&\quad + (1 + \alpha)\sum_{i=1}^{g} n_i^2 + (2 + \alpha)(1 + \alpha)\sum_{i=1}^{g} n_i \\
&= (1 + \alpha)\sum_{i=1}^{g} n_i^2 + \sum_{i=1}^{g} n_i n_{i+1} + (\alpha + 2)(\alpha + 3)(n - g) + (\alpha + 2)^2 g,
\end{aligned}$$

where $n_{g+1} = n_1$.

On the other hand, we have

$$\begin{aligned}
(1 + \alpha)\sum_{i=1}^{g} n_i^2 + \sum_{i=1}^{g} n_i n_{i+1} &= \left[\frac{1}{2}\sum_{i=1}^{g} n_i^2 + \sum_{i=1}^{g} n_i n_{i+1}\right] + \left(\frac{1}{2} + \alpha\right)\sum_{i=1}^{g} n_i^2 \\
&\leq \frac{1}{2}\left(\sum_{i=1}^{g} n_i\right)^2 + \left(\frac{1}{2} + \alpha\right)\left(\sum_{i=1}^{g} n_i\right)^2 \\
&= (1 + \alpha)(n - g)^2
\end{aligned} \tag{5}$$

as $\alpha \geq -\frac{1}{2}$. From Inequality (4) and Inequality (5), we get

$$\begin{aligned} GRM_\alpha(\Gamma) &\leq GRM_\alpha(\Gamma_0) \\ &= (1+\alpha)\sum_{i=1}^{g} n_i^2 + \sum_{i=1}^{g} n_i n_{i+1} + (\alpha+2)(\alpha+3)(n-g) + (\alpha+2)^2 g \\ &\leq (1+\alpha)(n-g)^2 + (\alpha+2)(\alpha+3)n - (\alpha+2)g. \end{aligned}$$

Suppose now that equality holds in (3). Then, the equality must hold in (5). Without loss of generality, we assume that $n_1 = \max\{n_1, n_2, \ldots, n_g\}$. Next, we distinguish the following three cases.

Case 1. $\alpha > -\frac{1}{2}$. From the equality in (5), we obtain $\sum\limits_{i=1}^{g} n_i^2 = \left(\sum\limits_{i=1}^{g} n_i\right)^2$, that is, $n_2 = n_3 = \cdots = n_g = 0$ as $n_1 \geq n_i$ for $1 \leq i \leq n$. So we have $\Gamma_0 \cong S(n-g, \underbrace{0, \ldots, 0}_{g-1})$. Additionally, by Lemma 2, one can easily check that

$$GRM_\alpha(\Gamma_0) = (1+\alpha)(n-g)^2 + (\alpha+2)(\alpha+3)n - (\alpha+2)g,$$

when $\Gamma_0 \cong S(n-g, \underbrace{0, \ldots, 0}_{g-1})$. Hence, the equality holds if, and only if, $\Gamma_0 \cong S(n-g, \underbrace{0, \ldots, 0}_{g-1})$.

Case 2. $\alpha = -\frac{1}{2}$ and $g \geq 4$. From the equality in (5), we obtain

$$\sum_{i=1}^{g} n_i^2 + 2\sum_{i=1}^{g} n_i n_{i+1} = \left(\sum_{i=1}^{g} n_i\right)^2, \tag{6}$$

that is,

$$\begin{aligned} 2n_1\sum_{i=2}^{g} n_i + \left(\sum_{i=2}^{g} n_i\right)^2 &= 2n_1(n_2+n_g) + 2(n_2n_3 + n_3n_4 + \cdots + n_{g-1}n_g) + \sum_{i=2}^{g} n_i^2 \\ &\leq 2n_1(n_2+n_g) + \left(\sum_{i=2}^{g} n_i\right)^2, \end{aligned}$$

that is,

$$n_1(n_3+n_4+\cdots+n_{g-1}) \leq 0 \quad \text{and hence} \quad n_1(n_3+n_4+\cdots+n_{g-1}) = 0. \tag{7}$$

If $n_1 = 0$, then $n_i = 0$ for all $1 \leq i \leq g$ (as $n_1 \geq n_i$ for all $1 \leq i \leq g$), that is, $\Gamma_0 \cong S(\underbrace{0, \ldots, 0}_{g})$ $(g = n)$, that is, $\Gamma_0 \in \mathcal{H}$. Otherwise, $n_1 > 0$. From (7), we obtain $n_3 + n_4 + \cdots + n_{g-1} = 0$, that is, $n_3 = n_4 = \cdots = n_{g-1} = 0$. From (6), we obtain

$$(n_1+n_2+n_g)^2 = n_1^2 + n_2^2 + n_g^2 + 2(n_1n_2 + n_gn_1), \quad \text{that is, } n_2n_g = 0.$$

Therefore, $n_2 = 0$ or $n_g = 0$. Without loss of generality, we can assume that $n_g = 0$. Hence the equality holds if, and only if, $n_1 + n_2 = n - g$, $n_1 \geq n_2$ and $n_3 = n_4 = \cdots = n_g = 0$. Hence $\Gamma_0 \in \mathcal{H}$.

Case 3. $\alpha = -\frac{1}{2}$ and $g = 3$. Then, the equality (5) holds clearly. Thus the equality holds in (3) if and only if $\Gamma_0 \in \{S(n_1, n_2, n_3) \mid n_1 \geq 0, n_2 \geq 0, n_3 \geq 0 \text{ and } n_1 + n_2 + n_3 = n-3\} \cong \mathcal{G}(n, n-3)$. This completes the proof. □

Corollary 1. *Let Γ be a unicyclic graph of order n with $\alpha \geq -\frac{1}{2}$. Then*

$$GRM_\alpha(\Gamma) \leq (1+\alpha)(n-3)^2 + (\alpha+2)(\alpha+3)n - 3(\alpha+2)$$

with equality if, and only if,
(i) $\Gamma \cong S(n-3,0,0)$ *when* $\alpha > -\frac{1}{2}$,
(ii) $\Gamma \in \mathcal{G}(n, n-3)$ *when* $\alpha = -\frac{1}{2}$.

Proof. Denote by g the girth of the graph Γ. Then, by Theorem 3 and $g \geq 3$, we have

$$\begin{aligned} GRM_\alpha(\Gamma) &\leq (1+\alpha)(n-g)^2 + (\alpha+2)(\alpha+3)n - (\alpha+2)g \\ &\leq (1+\alpha)(n-3)^2 + (\alpha+2)(\alpha+3)n - 3(\alpha+2) \end{aligned}$$

with equality if and only if
(i) $\Gamma \cong S(n-3,0,0)$ when $\alpha > -\frac{1}{2}$,
(ii) $\Gamma \in \mathcal{G}(n, n-3)$ when $\alpha = -\frac{1}{2}$.
By this, the proof is completed. □

Let $U(k_1, k_2, \ldots, k_g)$ be a unicyclic graph obtained from cycle $C_g = v_1 v_2 \ldots v_g v_1$ by joining an edge between the vertex v_i with a pendant vertex of a path P_{k_i} of length k_i, $i = 1, 2, \ldots, g$, that is, $U(k_1, k_2, \ldots, k_g) - E(C_g) \cong P_{k_1+1} \cup P_{k_2+1} \cup \cdots \cup P_{k_g+1}$. The graph $U(k_1, k_2, \ldots, k_g)$ has thus $n = g + \sum_{i=1}^{g} k_i$ vertices (see, Figure 3). By relabeling, we can assume that $k_1 = \max\{k_1, k_2, \ldots, k_g\}$. Let $\mathcal{U}(n, g)$ be a class of unicyclic graphs of order n with girth g ($n \geq g \geq 3$), is defined as

$$\mathcal{U}(n,g) = \left\{ U(k_1, k_2, \ldots, k_g) \mid \sum_{i=1}^{g} k_i = n - g \text{ and } k_1 \geq \max\{k_2, k_3, \ldots, k_g\} \right\}.$$

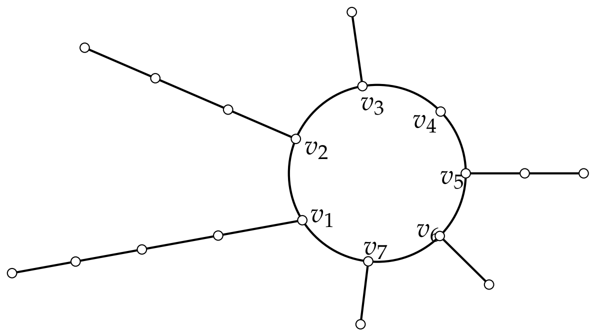

Figure 3. The graph $U(4,3,1,0,2,1,1)$ in $\mathcal{U}(19,7)$.

Repeating Transformation D, any tree T attached to a graph Γ can be changed into a path, as shown in Figure 4, and the general reduced second Zagreb index decreases when $\alpha \geq -\frac{1}{2}$ by Lemma 1. Thus, the next lemma follows immediately.

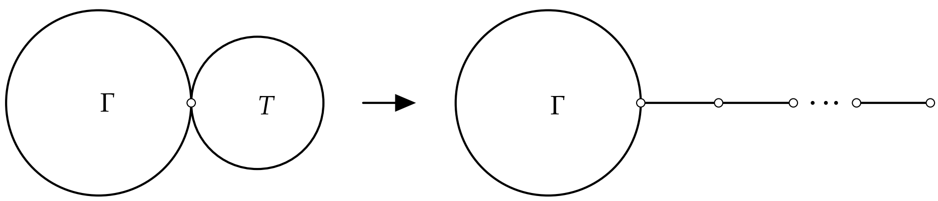

Figure 4. Repeating Transformation D.

Lemma 3. *Let $\Gamma \in \mathcal{U}_{n,g}$ with minimum GRM_α-value and $\alpha \geq -\frac{1}{2}$. Then $\Gamma \in \mathcal{U}(n,g)$.*

Theorem 4. *Let $\Gamma \in \mathcal{U}_{n,g}$ with minimum GRM_α-value and $\alpha \geq -\frac{1}{2}$. Then $\Gamma \cong U(n-g,\underbrace{0,\ldots,0}_{g-1})$.*

Proof. By Lemma 3, we have $\Gamma \in \mathcal{U}(n,g)$. So there exist non-negative integers $k_1, k_2, \ldots, k_g$ such that $\Gamma \cong U(k_1, k_2, \ldots, k_g)$. If $k_s \neq 0$ for $s \geq 2$, then we consider the graph $\Gamma_1 = U(k_1 + k_s, k_2, \ldots, k_{s-1}, 0, k_{s+1}, \ldots, k_g)$. By definition of GRM_α, we have

$$\begin{aligned} GRM_\alpha(\Gamma) - GRM_\alpha(\Gamma_1) &= (3+\alpha)(d_\Gamma(v_{s-1}) + d_\Gamma(v_{s+1}) + 2\alpha) + (2+\alpha)(1+\alpha) \\ &\quad + (3+\alpha)(2+\alpha) - (2+\alpha)(d_\Gamma(v_{s-1}) + d_\Gamma(v_{s+1}) + 2\alpha) - (2+\alpha)^2 - (2+\alpha)^2 \\ &= d_\Gamma(v_{s-1}) + d_\Gamma(v_{s+1}) + 2\alpha \geq d_\Gamma(v_{s-1}) + d_\Gamma(v_{s+1}) - 1 > 0 \end{aligned}$$

as $d_\Gamma(v_i) \geq 2$ for all $1 \leq i \leq g$. This is a contradiction that tells us $k_2 = k_3 = \cdots = k_g = 0$. The proof of the theorem is completed. □

An elementary calculation yields

$$GRM_\alpha\big(U(n-g,\underbrace{0,\ldots,0}_{g-1})\big) = \begin{cases} (n\alpha + 2n + 2)(2+\alpha) & \text{if } 3 \leq g \leq n-2, \\ (n\alpha + 2n + 2)(2+\alpha) - 1 & \text{if } g = n-1, \\ n(2+\alpha)^2 & \text{if } g = n. \end{cases} \tag{8}$$

Corollary 2. *Let Γ be a unicyclic graph of order n with $\alpha \geq -\frac{1}{2}$. Then*

$$GRM_\alpha(\Gamma) \geq n\,(2+\alpha)^2$$

with equality if, and only if, $\Gamma \cong C_n$.

4. Lower Bounds on GRM_α

Denote by $\mathcal{G}_n^{k+}$ and $\mathcal{G}_n^k$ the class of connected graphs of order n with at least k cut edges and the class of connected graphs of order n with exactly k cut edges. In [58], the extremal graphs with maximum GRM_α from $\mathcal{G}_n^{k+}$ and $\mathcal{G}_n^k$ were characterized. However, the extremal graphs with minimum GRM_α from $\mathcal{G}_n^{k+}$ and $\mathcal{G}_n^k$ were not characterized. In this section, we give the lower sharp bounds on GRM_α for these two classes of graphs. Let $\mathcal{G}'_{n,g}$ be the class of connected graphs of order n with girth g. All trees of order n belong to the class $\mathcal{G}_n^{k+}$ ($k = n-1$). The next two results immediately follow from our results in the previous section.

Theorem 5. *Let Γ be a graph in $\mathcal{G}_n^{k+}$ and $\alpha \geq -1/2$. Then*

$$GRM_\alpha(\Gamma) \geq (\alpha+2)(n+2\alpha-1)$$

with equality if, and only if,

$$\Gamma \cong \begin{cases} P_4 \text{ or } S_4 \;\; \text{when} \;\; n = 4 \;\; \text{and} \;\; \alpha = -\frac{1}{2}, \\ P_n \qquad \text{otherwise.} \end{cases}$$

Proof. Let $S \subset E(\Gamma)$ be a set of non-cut edges in Γ, such that $T = \Gamma - S$ is a tree. Then we have

$$GRM_\alpha(\Gamma) \geq GRM_\alpha(T) \geq (\alpha+2)(n+2\alpha-1)$$

by Proposition 1 and Theorem 2. Equality holding if, and only if, $\Gamma \cong T$ and

$$T \cong \begin{cases} P_4 \text{ or } S_4 & \text{if } \; n=4 \; \text{ and } \; \alpha = -\frac{1}{2}, \\ P_n & \text{otherwise.} \end{cases}$$

This completes the proof. □

Theorem 6. *Let Γ be a graph in $\mathcal{G}'_{n,g}$ and $\alpha \geq -1/2$. Then*

$$GRM_\alpha(\Gamma) \geq \begin{cases} (2+\alpha)(n\alpha+2n+2) & \text{if } 3 \leq g \leq n-2, \\ (2+\alpha)(n\alpha+2n+2)-1 & \text{if } g = n-1, \\ n\,(2+\alpha)^2 & \text{if } g=n \end{cases}$$

with equality if, and only if, $\Gamma \cong U(n-g, \underbrace{0,\ldots,0}_{g-1})$.

Proof. Let C be a cycle of length g in Γ. Let Γ' be a graph in $\mathcal{U}_{n,g}$, obtained by deleting the edges (which do not lie on the cycle C) of Γ. By Proposition 1, Theorem 4 and (8), we obtain

$$GRM_\alpha(\Gamma) \geq GRM_\alpha(\Gamma') \geq \begin{cases} (2+\alpha)(n\alpha+2n+2) & \text{if } 3 \leq g \leq n-2, \\ (2+\alpha)(n\alpha+2n+2)-1 & \text{if } g = n-1, \\ n\,(2+\alpha)^2 & \text{if } g=n. \end{cases}$$

Equality holding if, and only if, $\Gamma \cong \Gamma'$ and $\Gamma' \cong U(n-g, \underbrace{0,\ldots,0}_{g-1})$. □

We now consider cyclic graphs in $\mathcal{G}_n^{k+}$. Thus we have $k \leq n-2$, but there is no graph of order n with k cut edges if $k = n-2$. Therefore, we assume that $k \leq n-3$. Now, we characterize the extremal cyclic graphs from $\mathcal{G}_n^{k+}$ with minimum GRM_α using Theorem 6. Let $\mathcal{U}_n(k)$ be the set of all unicyclic graphs $U(t, \underbrace{0,\ldots,0}_{n-t-1})$, such that $k \leq t \leq n-3$. Because the number of cut edges in the graph Γ is at least k, we have the girth of Γ is at most $n-k$.

Theorem 7. *Let Γ be a cyclic graph from $\mathcal{G}_n^{k+}$ with minimum GRM_α. Let n, k be positive integers, such that $k \leq n-3$ and $\alpha \geq -\frac{1}{2}$. Then*
(i) $\Gamma \cong C_n$ if $k=0$.
(ii) $\Gamma \cong U(1, \underbrace{0,\ldots,0}_{n-1})$ if $k=1$.
(iii) $\Gamma \in \mathcal{U}_n(k)$ if $2 \leq k \leq n-3$.

Proof. Let g be the girth of Γ. Then, by Theorem 6, $\Gamma \cong U(n-g, \underbrace{0,\ldots,0}_{g-1})$, and we have Equation (8). Additionally, we have $g \leq n-k$ as $\Gamma \in \mathcal{G}_n^{k+}$. Hence, we obtain, easily, the required result and this completes the proof. □

Note that if $k \leq n-3$, then all graphs in $\mathcal{G}_n^k$ belong to the set of cyclic graphs in $\mathcal{G}_n^{k+}$ and $\mathcal{G}_n^k \cap \mathcal{U}_n(k) = \left\{ U(k, \underbrace{0,\ldots,0}_{n-k-1}) \right\}$. Therefore, we can obtain the following theorem that determines the extremal graphs of order n with k cut edges having minimum GRM_α when $\alpha \geq -\frac{1}{2}$.

Theorem 8. *Let Γ be a cyclic graph in $\mathcal{G}_n^k$ with minimum GRM_α and $\alpha \geq -\frac{1}{2}$, $k \leq n-3$. Then, $\Gamma \cong U(k, \underbrace{0, \ldots, 0}_{n-k-1})$.*

5. Upper Bounds on GRM_α

In this section, we give some upper bounds on the general reduced second Zagreb index GRM_α. Recall that a complete split graph $CS(n,\gamma)$ $(1 \leq \gamma \leq n-1)$ is defined as the graph join $\overline{K}_\gamma \vee K_{n-\gamma}$, where $\overline{K}_\gamma$ is the complement of the complete graph on γ vertices.

Theorem 9. *Let Γ be a graph of order n with independence number γ and $\alpha \geq -1$. Then*

$$GRM_\alpha(\Gamma) \leq (n-1+\alpha)^2 \binom{n-\gamma}{2} + (n-1+\alpha)(n-\gamma+\alpha)(n-\gamma)\gamma$$

with equality if, and only if, $\Gamma \cong CS(n,\gamma)$.

Proof. Let Γ_0 be a graph of order n with independence number γ and maximum GRM_α. Additionally, let S be an independent set in Γ_0 such that $|S| = \gamma$. If $\Gamma_0 \ncong CS(n,\gamma)$ then there exist non-adjacent vertices u and v so that $\{u,v\} \not\subset S$. For the graph $\Gamma_1 = \Gamma + uv$, the order is n and the independence number is γ. By Proposition 1, we have

$$GRM_\alpha(\Gamma_0) < GRM_\alpha(\Gamma_1)$$

and it is a contradiction to the fact that $GRM_\alpha(\Gamma_0)$ is maximum for the set of graphs of order n with independence number γ. Thus, we have $\Gamma_0 \cong CS(n,\gamma)$ and

$$GRM_\alpha(\Gamma) \leq GRM_\alpha(\Gamma_0).$$

One can easily check that

$$GRM_\alpha(CS(n,\gamma)) = (n-1+\alpha)^2 \binom{n-\gamma}{2} + (n-1+\alpha)(n-\gamma+\alpha)(n-\gamma)\gamma.$$

From this, the theorem is proved. □

Recall that $\mathcal{G}(n,r)$ is the set of graphs of order n with clique number $n-r$, and all the remaining r vertices are pendant. Denote by $\mathcal{P}_{n,r}$ the class of connected graphs of order n with r pendant vertices. Then, we have $\mathcal{G}(n,r) \subseteq \mathcal{P}_{n,r}$. For any graph Γ in $\mathcal{G}(n,r)$, there are some non-negative integers $k_1, k_2, \ldots, k_{n-r}$ such that $k_1 \geq k_2 \geq \cdots \geq k_{n-r}$, and the graph Γ is constructed by attaching k_i pendent vertices to the i-th vertex of a complete graph K_{n-r}, denoted $\Gamma(k_1, k_2, \ldots, k_{n-r})$ (see Figure 5). Clearly, we have $r = \sum_{i=1}^{n-r} k_i$.

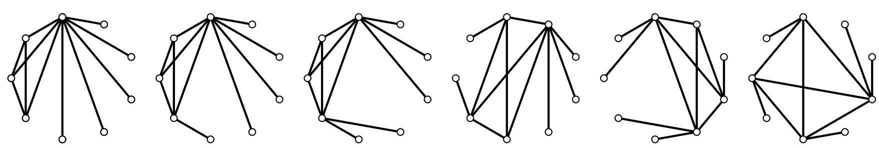

Figure 5. All graphs in $\mathcal{G}(9,5)$. For example, the fourth graph is denoted by $\Gamma(3,1,1,0)$.

Lemma 4. *Let Γ be a graph in $\mathcal{P}_{n,r}$ and $\alpha \geq -1$. If $GRM_\alpha(\Gamma)$ is maximum in $\mathcal{P}_{n,r}$ then $\Gamma \in \mathcal{G}(n,r)$.*

Proof. If $\Gamma \notin \mathcal{G}(n,r)$, then there exist two vertices u and v in Γ, such that $uv \notin E(\Gamma)$ and $d_\Gamma(u) > 1$, $d_\Gamma(v) > 1$. Denote by $\Gamma' = \Gamma + uv$. Then, $\Gamma' \in \mathcal{P}_{n,r}$ and by Proposition 1, we obtain $GRM_\alpha(\Gamma') > GRM_\alpha(\Gamma)$, a contradiction as $GRM_\alpha(\Gamma)$ is maximum in $\mathcal{P}_{n,r}$. Hence $\Gamma \in \mathcal{G}(n,r)$. $\square$

Theorem 10. *Let Γ be a graph with maximum GRM_α in $\mathcal{P}_{n,r}$ and $\alpha \geq -1$. Then*
(i) $\Gamma \cong \Gamma(k_1, k_2, \ldots, k_{n-r})$, where $\mid k_p - k_q \mid \leq 1$ for $1 \leq p, q \leq n-r$ if $-1 \leq \alpha \leq -\frac{1}{2}$.
(ii) $\Gamma \in \mathcal{G}(n,r)$ if $\alpha = -\frac{1}{2}$.
(iii) $\Gamma \cong \Gamma(r, \underbrace{0, \ldots, 0}_{n-k-1})$ if $\alpha > -\frac{1}{2}$.

Proof. By Lemma 4, we have $\Gamma \in \mathcal{G}(n,r)$. Therefore, $\Gamma \cong \Gamma(k_1, k_2, \ldots, k_{n-r})$ for some integers $k_1, k_2, \ldots, k_{n-r}$, such that $k_1 \geq k_2 \geq \cdots \geq k_{n-r} \geq 0$ and $r = \sum\limits_{i=1}^{n-r} k_i$. By the definition of GRM_α, we obtain

$$\begin{aligned}
GRM_\alpha(\Gamma) &= \sum_{1 \leq i < j \leq n-r} (n-r-1+k_i+\alpha)(n-r-1+k_j+\alpha) \\
&\quad + \sum_{i=1}^{n-r} k_i(1+\alpha)(n-r-1+k_i+\alpha) \\
&= \binom{n-r}{2}(n-r-1+\alpha)^2 + (n-r-1+\alpha) \sum_{1 \leq i < j \leq n-r} (k_i + k_j) \\
&\quad + \sum_{1 \leq i < j \leq n-r} k_i k_j + (1+\alpha)(n-r-1+\alpha) \sum_{i=1}^{n-r} k_i + (1+\alpha) \sum_{i=1}^{n-r} k_i^2 \\
&= \binom{n-r}{2}(n-r-1+\alpha)^2 + r(n-r-1+\alpha)(n-r+\alpha) \\
&\quad + (1+\alpha) \sum_{i=1}^{n-r} k_i^2 + \sum_{1 \leq i < j \leq n-r} k_i k_j \\
&= \binom{n-r}{2}(n-r-1+\alpha)^2 + r(n-r-1+\alpha)(n-r+\alpha) \\
&\quad + \left(\frac{1}{2} + \alpha\right) \sum_{i=1}^{n-r} k_i^2 + \frac{1}{2}\left(\sum_{i=1}^{n-r} k_i\right)^2 \\
&= \binom{n-r}{2}(n-r-1+\alpha)^2 + r(n-r-1+\alpha)(n-r+\alpha) \\
&\quad + \left(\frac{1}{2} + \alpha\right) \sum_{i=1}^{n-r} k_i^2 + \frac{1}{2} r^2. \qquad (9)
\end{aligned}$$

(i) Let $-1 \leq \alpha \leq -\frac{1}{2}$. Suppose that there are integers k_p and k_q such that $k_p - k_q \geq 2$. Then, we consider non-negative integers $k'_1, k'_2, \ldots, k'_{n-r}$ with $k'_p = k_p - 1$, $k'_q = k_q + 1$ and $k'_i = k_i$ for all $i \neq p, q$. Then we get

$$\sum_{i=1}^{n-r} k'^2_i - \sum_{i=1}^{n-r} k_i^2 = (k_p - 1)^2 + (k_q + 1)^2 - k_p^2 - k_q^2 = 2(k_q - k_p + 1) < 0.$$

Using this result in (9), we conclude that $GRM_\alpha(\Gamma)$ is not maximum as $-1 \leq \alpha \leq -\frac{1}{2}$. This is a contradiction. Hence $\Gamma \cong \Gamma(k_1, k_2, \ldots, k_{n-r})$, where $|k_p - k_q| \leq 1$ for $1 \leq p, q \leq n-r$.

(ii) Let $\alpha = -\frac{1}{2}$. Then

$$GRM_\alpha(\Gamma) = \binom{n-r}{2}(n-r-1+\alpha)^2 + r(n-r-1+\alpha)(n-r+\alpha) + \frac{1}{2} r^2.$$

Hence $\Gamma \in \mathcal{G}(n,r)$.

(iii) Let $\alpha > -\frac{1}{2}$. One can easily see that $\sum\limits_{i=1}^{n-r} k_i^2 \leq r^2$ with equality holding if, and only if, $k_1 = r$ and $k_2 = k_3 = \cdots = k_{n-r} = 0$. Using this result in (9), we obtain

$$GRM_\alpha(\Gamma) \leq \binom{n-r}{2}(n-r-1+\alpha)^2 + r(n-r-1+\alpha)(n-r+\alpha) + (\alpha+1)\, r^2$$

with equality if, and only if, $k_1 = r$ and $k_2 = k_3 = \cdots = k_{n-r} = 0$, that is, if, and only if, $\Gamma \cong \Gamma(r, \underbrace{0, \ldots, 0}_{n-k-1})$.

This completes the proof of the theorem. □

From Proposition 3, the following theorem is obtained.

Theorem 11. *Let Γ be a K_{r+1}-free graph of order n with m edges. Additionally, let n, r be positive integers and α be real number, such that $2 \leq r \leq n-1$ and $\frac{r-2}{2r}n + \alpha \geq 0$. Then*

$$GRM_\alpha(\Gamma) \leq \frac{2}{r}m^2 + \left(\frac{r-2}{2r}n + \alpha\right) \cdot \frac{2r-2}{r}mn + \alpha^2 m \tag{10}$$

with equality if, and only if, Γ is isomorphic to a regular complete r-partite graph for $r \geq 3$ and a complete bipartite graph for $r = 2$.

Proof. From the definition of GRM_α with Proposition 3, we obtain

$$\begin{aligned} GRM_\alpha(\Gamma) &= M_2(\Gamma) + \alpha M_1(\Gamma) + \alpha^2 m \leq \frac{2}{r}m^2 + \left(\frac{r-2}{2r}n + \alpha\right) \cdot M_1(\Gamma) + \alpha^2 m \\ &\leq \frac{2}{r}m^2 + \left(\frac{r-2}{2r}n + \alpha\right) \cdot \frac{2r-2}{r}mn + \alpha^2 m \end{aligned}$$

as $\frac{r-2}{2r}n + \alpha \geq 0$. Moreover, the equality holds in (10) if, and only if, Γ is isomorphic to a complete bipartite graph for $r = 2$ and a regular complete r-partite graph for $r \geq 3$. This completes the proof. □

Note that if $r \geq 4$ or $r = 3$ and $n \geq 6$ then for all $\alpha \geq -1$, Theorem 11 holds as $\frac{r-2}{2r}n + \alpha \geq 0$. Moreover, for all $\alpha \geq -1$, the following theorem, which is a generalization of Theorem 2.3 in [57] holds. Denote Γ_4 the graph of order 4 with size 1.

Theorem 12. *Let Γ be a K_{r+1}-free graph with n vertices $(3 \leq r \leq n-1)$ and $m > 0$ edges. If $\alpha \geq -1$ and $\Gamma \ncong \Gamma_4$, then*

$$GRM_\alpha(\Gamma) \leq \frac{2}{r}m^2 + \left(\frac{r-2}{2r}n + \alpha\right) \cdot \frac{2r-2}{r}mn + \alpha^2 m \tag{11}$$

with equality if, and only if, Γ is isomorphic to a regular complete r-partite graph.

Proof. If $r \geq 4$, or $r = 3$ and $n \geq 6$, then we obtain $\frac{r-2}{2r}n + \alpha \geq \frac{r-2}{2r}n - 1 \geq 0$ and by Theorem 11, the proof is finished. Hence, we have only the following two cases.

Case 1. $n = 4$ and $r = 3$. The right-hand side of (11) is equal to $\frac{2}{3}m^2 + \left(\frac{2}{3} + \alpha\right) \cdot \frac{16}{3}m + \alpha^2 m$. For $m = 1$, it contradicts the assumption that Γ is not isomorphic to Γ_4. For $m = 2$, we have $\Gamma \cong K_2 \cup K_2$ or $\Gamma \cong K_{1,2} \cup K_1$. Then

$$GRM_\alpha(\Gamma) \leq 2(1+\alpha)(2+\alpha) < \frac{2}{3}m^2 + \left(\frac{2}{3} + \alpha\right) \cdot \frac{16}{3}m + \alpha^2 m$$

as $\alpha \geq -1$. Let now $m \geq 3$. If $\Delta(\Gamma) \leq 2$, then

$$GRM_\alpha(\Gamma) \leq (2+\alpha)(2+\alpha)m < \frac{2}{3}m^2 + \left(\frac{2}{3}+\alpha\right) \cdot \frac{16}{3}m + \alpha^2 m$$

as $m \geq 3$ and $\alpha \geq -1$. Otherwise, $\Delta(\Gamma) = 3$. Then, there are only three K_4-free graphs, which are $K_{1,3}$, $K_{1,3}+e$ and $K_4 - e$, and for these graphs the strict inequality in (11) holds.

Case 2. $n = 5$ and $r = 3$. The right-hand side of (11) is equal to $\frac{2}{3}m^2 + \left(\frac{5}{6}+\alpha\right) \cdot \frac{20}{3}m + \alpha^2 m$. For $m = 1$, we have $GRM_\alpha(\Gamma) = (1+\alpha)^2 < \frac{2}{3}m^2 + \left(\frac{5}{6}+\alpha\right) \cdot \frac{20}{3}m + \alpha^2 m$. Let now $m \geq 2$. For $\Delta(\Gamma) \leq 2$, we obtain

$$GRM_\alpha(\Gamma) \leq m(2+\alpha)(2+\alpha) < \frac{2}{3}m^2 + \left(\frac{5}{6}+\alpha\right) \cdot \frac{20}{3}m + \alpha^2 m$$

as $m \geq 2$ and $\alpha \geq -1$. Let $\Delta(\Gamma) = 3$. Then clearly $m \geq 3$. For $m = 3$, Γ is $K_{1,3} + K_1$. If there is a graph H of order 4 such that Γ is $H + K_1$, then by the previous case, we have

$$\begin{aligned} GRM_\alpha(\Gamma) = GRM_\alpha(H) &< \frac{2}{3}m^2 + \left(\frac{2}{3}+\alpha\right) \cdot \frac{16}{3}m + \alpha^2 m \\ &< \frac{2}{3}m^2 + \left(\frac{5}{6}+\alpha\right) \cdot \frac{20}{3}m + \alpha^2 m \end{aligned}$$

as $\alpha \geq -1$. For $m = 4$, Γ is the fork graph. Of course, the strict inequality in (11) holds for the fork. Let $m \geq 5$. Then Γ has at least one vertex of degree less than three by the handshaking lemma. Hence

$$\begin{aligned} GRM_\alpha(\Gamma) &\leq (3+\alpha)(3+\alpha)(m-2) + (3+\alpha)(2+\alpha) \cdot 2 \\ &< \frac{2}{3}m^2 + \left(\frac{5}{6}+\alpha\right) \cdot \frac{20}{3}m + \alpha^2 m \end{aligned}$$

as $m \geq 5$ and $\alpha \geq -1$.

Let now $\Delta(\Gamma) = 4$. If $m = 4$ or $m = 5$, then Γ is $K_{1,4}$ or $K_{1,4} + e$. For $m \geq 6$, all K_4- free graphs of order 5 with m edges and maximum degree 4 are displayed in Figure 6. One can easily check that the strict inequality in (11) holds for all of the graphs in Figure 6. □

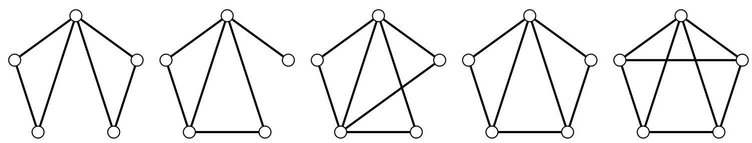

Figure 6. All K_4- free graphs of order 5 with m ($m \geq 6$) edges and $\Delta = 4$.

Corollary 3. *Let Γ be a K_{r+1}-free graph with n vertices ($3 \leq r \leq n-1$) and $m > 0$ edges. If $\alpha \geq -\frac{29}{30}$, then*

$$GRM_\alpha(\Gamma) \leq \frac{2}{r}m^2 + \left(\frac{r-2}{2r}n + \alpha\right) \cdot \frac{2r-2}{r}mn + \alpha^2 m$$

with equality if, and only if, Γ is isomorphic to a regular complete r-partite graph.

We give now an upper bound on GRM_α, which is a generalization of Theorem 2.5 in [57] for the class of triangle-free graphs.

Theorem 13. *Let Γ be a connected triangle-free graph of order $n > 2$ with $m > 0$ edges and $\alpha > -1.5$. Then*

$$GRM_\alpha(\Gamma) \le \left(\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil + n\alpha + \alpha^2\right) m \tag{12}$$

with equality if, and only if, $\Gamma \cong T_n(2)$.

Proof. Let uv be an edge in Γ such that $(d_\Gamma(u)+\alpha)(d_\Gamma(v)+\alpha)$ is maximum. Since Γ is triangle free, we have $N_\Gamma(u) \cap N_\Gamma(v) = \emptyset$, which means that $d_\Gamma(u) + d_\Gamma(v) \le n$. Therefore

$$\begin{aligned} GRM_\alpha(\Gamma) &= \sum_{u_iv_j \in E(\Gamma)} (d_\Gamma(u_i)+\alpha)(d_\Gamma(v_j)+\alpha) \\ &\le m(d_\Gamma(u)+\alpha)(d_\Gamma(v)+\alpha) \qquad (13) \\ &= m\Big(d_\Gamma(u)d_\Gamma(v) + (d_\Gamma(u)+d_\Gamma(v))\,\alpha + \alpha^2\Big) \\ &\le m\left(\left\lfloor \frac{d_\Gamma(u)+d_\Gamma(v)}{2} \right\rfloor \left\lceil \frac{d_\Gamma(u)+d_\Gamma(v)}{2} \right\rceil + (d_\Gamma(u)+d_\Gamma(v))\,\alpha + \alpha^2\right). \qquad (14) \end{aligned}$$

Let us consider a function

$$f(x) = \left\lfloor \frac{x}{2} \right\rfloor \left\lceil \frac{x}{2} \right\rceil + x\alpha,\ 3 \le x \le n.$$

One can easily see that

$$f(x+1) - f(x) = \begin{cases} \dfrac{x}{2} + \alpha & \text{if } x \text{ is even,} \\ \dfrac{x+1}{2} + \alpha & \text{if } x \text{ is odd.} \end{cases}$$

Since $3 \le x \le n$ and $\alpha > -1.5$, we have $f(x+1) - f(x) > 0$, that is,

$$f(3) < f(4) < \cdots < f(n-1) < f(n) = \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil + n\alpha.$$

Since Γ is connected and $n > 2$, we have $3 \le d_\Gamma(u) + d_\Gamma(v) \le n$. Using these results in (14), we obtain

$$GRM_\alpha(\Gamma) \le \left(\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil + n\alpha + \alpha^2\right) m.$$

The first part of the proof is done.

Suppose now that equality holds in (12). Then, all inequalities in the above must be equalities. From the equality in (13), we have

$$(d_\Gamma(u_i)+\alpha)(d_\Gamma(v_j)+\alpha) = (d_\Gamma(u)+\alpha)(d_\Gamma(v)+\alpha) \ \text{ for any edge } \ u_iv_j \in E(\Gamma). \tag{15}$$

From the equality in (14), we have

$$d_\Gamma(u)d_\Gamma(v) = \left\lfloor \frac{d_\Gamma(u)+d_\Gamma(v)}{2} \right\rfloor \left\lceil \frac{d_\Gamma(u)+d_\Gamma(v)}{2} \right\rceil.$$

Moreover, we have $d_\Gamma(u) + d_\Gamma(v) = n$. Thus, we have $d_\Gamma(u)d_\Gamma(v) = \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$. From this we conclude that $\big(d_\Gamma(u), d_\Gamma(v)\big) = (\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil)$ or $\big(d_\Gamma(u), d_\Gamma(v)\big) = (\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor)$. Let u_i be any vertex in Γ which is different from u and v. Then u_i is adjacent to either u or v, because Γ is triangle free and $d_\Gamma(u) + d_\Gamma(v) = n$. Suppose that $u_i \in N_\Gamma(u)$. Then, all neighbors of u_i are adjacent to v as Γ is triangle-free and $d_\Gamma(u) + d_\Gamma(v) = n$. Hence $d_\Gamma(u_i) \le d_\Gamma(v)$. If v_j is any vertex adjacent to u_i, then $v_j v \in E(\Gamma)$. Similarly, we get $d_\Gamma(v_j) \leq d_\Gamma(u)$. From (15), we have $d_\Gamma(u_i) = d_\Gamma(v)$ and $d_\Gamma(v_j) = d_\Gamma(u)$. Hence $\Gamma \cong T_n(2)$.

Conversely, let $\Gamma \cong T_n(2)$. Then

$$GRM_\alpha(\Gamma) = \left(\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil + n\alpha + \alpha^2 \right) m.$$

□

Let $\mathcal{X}_{n,k}$ be the set of graphs of order n with chromatic number k. In [57,60], the extremal graphs of order n with chromatic number k respect to M_2 and RM_2 were characterized. We now generalize these results. From the definition of $\mathcal{X}_{n,k}$ and Proposition 1, we obtain, easily, the following lemma.

Lemma 5. *Let $\Gamma \in \mathcal{X}_{n,k}$ be a graph with maximal $GRM_\alpha(\Gamma)$ and $\alpha \geq -1$. Then $\Gamma \cong K_{n_1,n_2,\ldots,n_k}$.*

Theorem 14. *Let $\Gamma \in \mathcal{X}_{n,k}$ and $\alpha \geq -1$. If $GRM_\alpha(\Gamma)$ is maximum in $\mathcal{X}_{n,k}$, then $\Gamma \cong T_n(k)$.*

Proof. Let $\Gamma \in \mathcal{X}_{n,k}$ such that $GRM_\alpha(\Gamma)$ is maximum. From Lemma 5, $\Gamma \cong K_{n_1,n_2,\ldots,n_k}$. By contradiction we prove that $\Gamma \cong T_n(k)$. For this we assume that $K_{n_1,n_2,\ldots,n_k} \ncong T_n(k)$. Then, there are two parts of the partitions in $K_{n_1,n_2,\ldots,n_k}$ whose sizes are n_p and n_q, such that $n_q - n_p \geq 2$ for $1 \leq p < q \leq k$.

Consider the complete k-partite graph $\Gamma' \cong K_{n_1,\ldots,n_{p-1},n_p+1,n_{p+1}\ldots,n_{q-1},n_q-1,n_{q+1}\ldots,n_k}$ and by definition of GRM_α, we have

$$GRM_\alpha(\Gamma') - GRM_\alpha(\Gamma) = M_2(\Gamma') - M_2(\Gamma) + \alpha\big(M_1(\Gamma') - M_1(\Gamma)\big) + \alpha^2\big(m(\Gamma') - m(\Gamma)\big).$$

From Proposition 4, we have

$$M_1(\Gamma') - M_1(\Gamma) > 0 \text{ and } \Delta M(\Gamma') - \Delta M(\Gamma) > 0.$$

Additionally, by the definition of a complete k-partite graph, we have

$$\begin{aligned} 2m(\Gamma') - 2m(\Gamma) &= (n - n_q + 1)(n_q - 1) + (n - n_p - 1)(n_p + 1) \\ &\quad - (n - n_p)n_p - (n - n_q)n_q \\ &= 2(n_q - n_p - 1) > 0. \end{aligned}$$

Thus, we obtain

$$\begin{aligned} & GRM_\alpha(\Gamma') - GRM_\alpha(\Gamma) \\ = {} & M_2(\Gamma') - M_2(\Gamma) + \alpha\big(M_1(\Gamma') - M_1(\Gamma)\big) + \alpha^2\big(m(\Gamma') - m(\Gamma)\big) \\ \geq {} & M_2(\Gamma') - M_2(\Gamma) - \big(M_1(\Gamma') - M_1(\Gamma)\big) + \alpha^2\big(m(\Gamma') - m(\Gamma)\big) \\ = {} & \Delta M(\Gamma') - \Delta M(\Gamma) + \alpha^2\big(m(\Gamma') - m(\Gamma)\big) > 0. \end{aligned}$$

This is contradicts the fact that $GRM_\alpha(\Gamma)$ is maximum. Hence $\Gamma \cong T_n(k)$ and the proof is completed. □

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