Improved lower bounds on the general reduced second Zagreb index of trees

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Abstract

For a graph Γ , the general reduced second Zagreb index is defined as

$$GRM_{\lambda}(\Gamma) = \sum_{ab \in E(\Gamma)} \left[(\deg_{\Gamma}(a) + \lambda) (\deg_{\Gamma}(b) + \lambda) \right],$$

where λ is an arbitrary real number and $\deg_{\Gamma}(a)$ is the degree of the vertex a. Buyantogtokh et al. showed that if T is a tree of order n and $\lambda \geq -\frac{1}{2}$, then $GRM_{\lambda}(T) \geq (\lambda+2)(n-2\lambda-1)$. We improve this result by proving that if T is a tree of order $n \geq 4$, $\lambda \geq -1$, and $\Delta = \Delta(T)$, then

$$GRM_{\lambda}(T) \geqslant \begin{cases} (n\lambda + 2n - \Delta\lambda - \Delta - 3)(2 + \lambda) + (\Delta - 1)(\Delta + \lambda)(1 + \lambda); & \Delta < n - 1, \\ \Delta(\Delta + \lambda)(1 + \lambda); & \Delta = n - 1. \end{cases}$$

The corresponding extremal trees are also determined.

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1 Introduction

Consider a graph $\Gamma = (V(\Gamma), E(\Gamma))$. For $a \in V(\Gamma)$, the open neighborhood $N_{\Gamma}(a)$ of a in Γ is the set $N_{\Gamma}(a) = \{b \in V(\Gamma) \mid ab \in E(\Gamma)\}$. The degree of a in Γ is deg_{Γ} $(a) = |N_{\Gamma}(a)|$. The maximum degree of Γ is denoted by $\Delta(\Gamma)$. The distance between the vertices $a, b \in V(\Gamma)$, $d_T(a, b)$, is the length of a shortest a, b-path in Γ .

The first Zagreb index [15] and the second Zagreb index [14] are the oldest members of the nowadays rich family of vertex-degree-based indices, and are respectively defined as

$$M_1(\Gamma) = \sum_{a \in V(\Gamma)} \deg_{\Gamma}(a)^2$$
 and $M_2(\Gamma) = \sum_{ab \in E(\Gamma)} \deg_{\Gamma}(a) \deg_{\Gamma}(b)$

For comprehensive, transparent information on these indices we refer to [2, 6, 13]. However, research is still intensively ongoing, the papers [1, 18, 20, 22] are instances of the latest developments. Moreover, in the last decade different vertex-degree-based indices were proposed such as atom-bond connectivity index [10], sum connectivity index [24], irregularity [3, 5], Lanzhou index [9, 23], and entire Zagreb indices [4, 19].

Furtula et al. [11] showed that the difference $M_2(\Gamma) - M_1(\Gamma)$ is closely related to the reduced second Zagreb index $RM_2(\Gamma)$ which is defined as

$$RM_2(\Gamma) = \sum_{ab \in E(\Gamma)} \left[(\deg_{\Gamma}(a) - 1)(\deg_{\Gamma}(b) - 1) \right],$$

and was studied in many papers, cf. [8, 12, 21].

In 2019, Horoldagva et al. [16] extended the reduced second Zagreb index to the general reduced second Zagreb index $GRM_{\lambda}(\Gamma)$ as

$$GRM_{\lambda}(\Gamma) = \sum_{ab \in E(\Gamma)} \left[(\deg_{\Gamma}(a) + \lambda)(\deg_{\Gamma}(b) + \lambda) \right],$$

where λ is an arbitrary real number. This definition can be equivalently stated as $GRM_{\lambda}(\Gamma) = M_2(\Gamma) + \lambda M_1(\Gamma) + \lambda^2 |E(\Gamma)|$. Even this very general version has already received a considerable interest [7, 16, 17].

Our primary motivation for the present paper is the following result, which has been demonstrated by Buyantogtokh et al. in [7].

Theorem A. If T be a tree of order n, and $\lambda \geq -\frac{1}{2}$, then

$$GRM_{\lambda}(T) \ge (\lambda + 2)(n - 2\lambda - 1),$$

with equality if and only if $T = P_4$ or $T = S_4$ when n = 4 and $\lambda = -\frac{1}{2}$, and $T = P_n$ otherwise.

In this paper we extend the bound of Theorem A by establishing a sharp lower bound for the general reduced second Zagreb index of trees of given order and maximum degree. We also determine the extremal trees achieving this bound. The results and their proofs are presented in the next section, where we will need the next result.

Theorem B. [16] If Γ be a connected graph and $\lambda \geq -1$, then for every edge $e \notin E(\Gamma)$, $GRM_{\lambda}(\Gamma + e) > GRM_{\lambda}(\Gamma)$.

2 The bound

A rooted tree is a tree together with a special vertex chosen as the root of the tree. A spider is a tree with exactly one vertex of degree more than two. The high degree vertex of a spider T is the *center* of T. A leg of a spider is a path from its center to a leaf. A star is a spider with all legs of length one. In needed and by abuse of language we also consider a path graph to be a spider (with one or two leg).

For positive integers n and Δ , let $\mathcal{T}_{n,\Delta}$ be the set of all trees of order n and maximum degree Δ . Then the key lemma for our announced inequality reads as follows.

Lemma 1. Let $\lambda \geq -1$, $\Delta \geq 3$, $T \in \mathcal{T}_{n,\Delta}$, and let a be a vertex of T with $\deg_T(a) = \Delta$. If T contains a vertex $b \neq a$ with $\deg_T(b) \geq 3$, then there exists a tree $T^* \in \mathcal{T}_{n,\Delta}$ such that $GRM_{\lambda}(T^*) < GRM_{\lambda}(T)$.

Proof. Consider T as a rooted tree with the root a. We may without loss of generality assume that among all vertices $x \neq a$ with $\deg_T(x) \geq 3$, the vertex b has maximum distance to a. Let $\deg_T(b) = \ell$, and let $N_T(b) = \{b_1, \ldots, b_\ell\}$, where b_ℓ is the neighbor of b that lies on the b, a-path in T. By our assumption on $d_T(a, b)$ we have $\deg_T(b_i) \in \{1, 2\}$ for each $i \in [\ell - 1]$. Based on the latter degrees, we distinguish the following three cases.

Case 1: *b* is adjacent to at least two leaves.

We may without loss of generality assume that b_1 and b_2 are leaves. Let T^* be the tree obtained from T by removing the vertex b_1 and adding the edge b_1b_2 . That is, in T^* the vertex b_2 becomes the support vertex of the leaf b_1 . See Fig. 1.

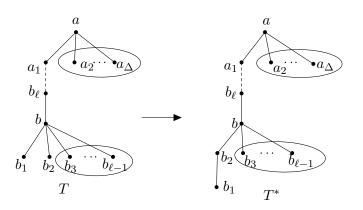


Figure 1: Transformation from Case 1

Recall that $\lambda \geq -1$ and $\ell \geq 3$. If we put $X = GRM_{\lambda}(T) - GRM_{\lambda}(T^*)$, then we can calculate as follows:

$$X = \deg_T(b) + \lambda)(\deg_T(b_1) + \lambda) + (\deg_T(b) + \lambda)(\deg_T(b_2) + \lambda)$$

$$\begin{aligned} &+ (\deg_T(b) + \lambda)(\deg_T(b_\ell) + \lambda) + \sum_{i=3}^{\ell-1} (\deg_T(b) + \lambda)(\deg_T(b_i) + \lambda) \\ &- (\deg_{T^*}(b_1) + \lambda)(\deg_{T^*}(b_2) + \lambda) - (\deg_{T^*}(b) + \lambda)(\deg_{T^*}(b_2) + \lambda) \\ &- (\deg_{T^*}(b) + \lambda)(\deg_{T^*}(b_\ell) + \lambda) - \sum_{i=3}^{\ell-1} (\deg_{T^*}(b) + \lambda)(\deg_{T^*}(b_i) + \lambda) \\ &= 2(1 + \lambda)(\ell + \lambda) + (\ell + \lambda)(\deg_T(b_\ell) + \lambda) \\ &+ \sum_{i=3}^{\ell-1} (\ell + \lambda)(\deg_T(b_i) + \lambda) \\ &- (1 + \lambda)(2 + \lambda) - (2 + \lambda)(\ell - 1 + \lambda) - (\ell - 1 + \lambda)(\deg_T(b_\ell) + \lambda) \\ &- \sum_{i=3}^{\ell-1} (\ell - 1 + \lambda)(\deg_T(b_i) + \lambda) \\ &= \lambda^2 + 2\lambda + \deg_T(b_\ell) + 2 + \sum_{i=3}^{\ell-1} (\deg_T(b_i) + \lambda) \\ &\geq \lambda^2 + 2\lambda + \deg_T(b_\ell) + 2 > 0. \end{aligned}$$

Case 2: *b* is adjacent to exactly one leaf.

We may assume that b_1 is the leaf adjacent to b. Let $bc_1c_2...c_k$, be the path in T where $b_2 = c_1, k \ge 2$, and c_k is a leaf. Let T^* be the tree obtained from T by removing the vertex b_1 and path $c_1c_2...c_k$ and attaching to b the path $c_1c_2...c_kb_1$. See Fig. 2.

Using the fact that $\lambda \geq -1$ and $\ell \geq 3$, and putting $X = GRM_{\lambda}(T) - GRM_{\lambda}(T^*)$, we have:

$$\begin{split} X &= (\deg_T(b) + \lambda)(\deg_T(b_1) + \lambda) + (\deg_T(c_k) + \lambda)(\deg_T(c_{k-1}) + \lambda) \\ &+ (\deg_T(b) + \lambda)(\deg_T(b_\ell) + \lambda) + \sum_{i=2}^{\ell-1} (\deg_T(b) + \lambda)(\deg_T(b_i) + \lambda) \\ &- (\deg_{T^*}(b_1) + \lambda)(\deg_{T^*}(c_k) + \lambda) - (\deg_{T^*}(c_k) + \lambda)(\deg_{T^*}(c_{k-1}) + \lambda) \\ &- (\deg_{T^*}(b) + \lambda)(\deg_{T^*}(b_\ell) + \lambda) - \sum_{i=2}^{\ell-1} (\deg_{T^*}(b) + \lambda)(\deg_{T^*}(b_i) + \lambda) \\ &= (1 + \lambda)(\ell + \lambda) + (1 + \lambda)(2 + \lambda) + (\ell + \lambda)(\deg_T(b_\ell) + \lambda) \\ &+ \sum_{i=2}^{\ell-1} (\ell + \lambda)(\deg_T(b_i) + \lambda) \\ &- (1 + \lambda)(2 + \lambda) - (2 + \lambda)^2 - (\ell - 1 + \lambda)(\deg_T(b_\ell) + \lambda) \end{split}$$

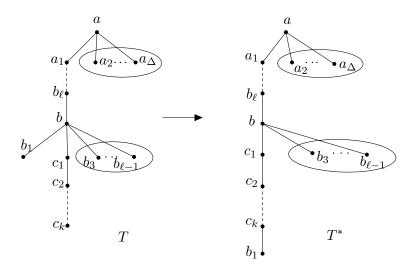


Figure 2: The construction from Case 2

$$-\sum_{i=2}^{\ell-1} (\ell - 1 + \lambda) (\deg_T(b_i) + \lambda)$$
$$= \ell \lambda + \ell + \deg_T(b_\ell) - 2\lambda - 4 + \sum_{i=2}^{\ell-1} (\deg_T(b_i) + \lambda)$$
$$> \ell \lambda + \ell + \deg_T(b_\ell) - 2\lambda - 4 \ge 0.$$

Case 3: None of the vertices adjacent to *b* is a leaf.

Let $bc_1c_2...c_k$ and $bd_1d_2...d_s$ be the paths in T such that $k, s \ge 2, b_1 = c_1, b_2 = d_1$, and c_k and d_s are leaves. Let T^* be the tree obtained from T achieved by removing the path $c_1...c_k$ and attaching it to d_s , see Fig. 3.

Once more setting $X = GRM_{\lambda}(T) - GRM_{\lambda}(T^*)$, we can estimate as follows:

$$\begin{split} X &= (\deg_T(b) + \lambda)(\deg_T(b_1) + \lambda) + (\deg_T(d_s) + \lambda)(\deg_T(d_{s-1}) + \lambda) \\ &+ (\deg_T(b) + \lambda)(\deg_T(b_\ell) + \lambda) + \sum_{i=2}^{\ell-1} (\deg_T(b) + \lambda)(\deg_T(b_i) + \lambda) \\ &- (\deg_{T^*}(b_1) + \lambda)(\deg_{T^*}(d_s) + \lambda) - (\deg_{T^*}(d_s) + \lambda)(\deg_{T^*}(d_{s-1}) + \lambda) \\ &- (\deg_{T^*}(b) + \lambda)(\deg_{T^*}(b_\ell) + \lambda) - \sum_{i=2}^{\ell-1} (\deg_{T^*}(b) + \lambda)(\deg_{T^*}(b_i) + \lambda) \\ &= (2 + \lambda)(\ell + \lambda) + (1 + \lambda)(2 + \lambda) + (\ell + \lambda)(\deg_T(b_\ell) + \lambda) \end{split}$$

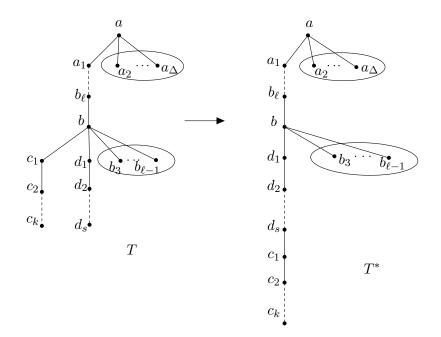


Figure 3: Transformation in Case 3

$$+\sum_{i=2}^{\ell-1} (\ell+\lambda)(\deg_T(b_i)+\lambda)$$
$$-(1+\lambda)(2+\lambda) - (2+\lambda)^2 - (\ell-1+\lambda)(\deg_T(b_\ell)+\lambda)$$
$$-\sum_{i=2}^{\ell-1} (\ell-1+\lambda)(\deg_T(b_i)+\lambda)$$
$$= \ell\lambda + \ell + \deg_T(b_\ell) - 2\lambda - 4 + \sum_{i=2}^{\ell-1} (\deg_T(b_i)+\lambda)$$
$$> \ell\lambda + 2\ell + \deg_T(b_\ell) - 2\lambda - 6 > 0.$$

This completes the proof of Lemma 1.

Our second lemma deals with spiders.

Lemma 2. If $T \in \mathcal{T}_{n,\Delta}$ is a spider with $\Delta \geq 3$ such that T has two legs of length more than one, then there is a spider $T^* \in \mathcal{T}_{n,\Delta}$ such that $GRM_{\lambda}(T^*) < GRM_{\lambda}(T)$.

Proof. Let a be the center of T, and let $ab_1 \dots b_t$ and $ac_1 \dots c_k$ be two legs of length more than one in T. Let T^* be the tree obtained from T by removing the path $b_2 \dots b_t$ and attaching it

in T^* to c_k . If $X = GRM_{\lambda}(T) - GRM_{\lambda}(T^*)$, then

$$\begin{split} X &= (\deg_T(a) + \lambda)(\deg_T(b_1) + \lambda) + (\deg_T(b_1) + \lambda)(\deg_T(b_2) + \lambda) \\ &+ (\deg_T(c_k) + \lambda)(\deg_T(c_{k-1}) + \lambda) \\ &- (\deg_{T^*}(a) + \lambda)(\deg_{T^*}(b_1) + \lambda) - (\deg_{T^*}(c_k) + \lambda)(\deg_{T^*}(c_{k-1}) + \lambda) \\ &- (\deg_{T^*}(b_2) + \lambda)(\deg_{T^*}(c_k) + \lambda) \\ &= (2 + \lambda)(\Delta + \lambda) + (2 + \lambda)(\deg_T(b_2) + \lambda) + (1 + \lambda)(2 + \lambda) \\ &- (1 + \lambda)(\Delta + \lambda) - (\deg_{T^*}(b_2) + \lambda)(2 + \lambda) - (2 + \lambda)^2 \\ &= \Delta - 2 > 0, \end{split}$$

and we are done.

Now we can prove the main results of this paper.

Theorem 3. If $\lambda \geq -1$, $n \geq 4$, and $T \in \mathcal{T}_{n,\Delta}$, then

$$GRM_{\lambda}(T) \geqslant \begin{cases} (n\lambda + 2n - \Delta\lambda - \Delta - 3)(2 + \lambda) + (\Delta - 1)(\Delta + \lambda)(1 + \lambda); & \Delta < n - 1, \\ \\ \Delta(\Delta + \lambda)(1 + \lambda); & \Delta = n - 1. \end{cases}$$

The equality holds if T is a spider with at most one leg of length more than one.

Proof. Let T^* be a tree from $\mathcal{T}_{n,\Delta}$ such that $GRM_{\lambda}(T^*) \leq GRM_{\lambda}(T)$ for all $T \in \mathcal{T}_{n,\Delta}$. Consider T^* rooted at a, where $\deg_{T^*}(a) = \Delta$. If $\Delta = 2$, then T is a path of order $n \geq 4$ and $GRM_{\lambda}(T) = (n-3)(2+\lambda)^2 + 2(1+\lambda)(2+\lambda)$. Thus let $\Delta \geq 3$. Then by Lemma 1, T^* is a spider with center a and by Lemma 2, T^* has at most one leg of length more than one. If all legs of T^* have length one, then T^* is a star and $GRM_{\lambda}(T^*) = (n-1)(1+\lambda)(n-1+\lambda)$. Assume hence that T^* is not a star and that T^* has only one leg of length more than one. Then

$$GRM_{\lambda}(T) \ge (n - \Delta - 2)(2 + \lambda)^{2} + (\Delta - 1)(\Delta + \lambda)(1 + \lambda) + (\Delta + \lambda)(2 + \lambda) + (1 + \lambda)(2 + \lambda),$$

and the proof is complete.

If $\lambda \ge -\frac{1}{2}$, $n \ge 6$, and $3 < \Delta < n - 1$, then

$$(n\lambda + 2n - \Delta\lambda - \Delta - 3)(2 + \lambda) + (\Delta - 1)(\Delta + \lambda)(1 + \lambda) - (\lambda + 2)(n - 2\lambda - 1)$$

= $(n\lambda + n - \Delta\lambda - \Delta + 2\lambda - 2)(2 + \lambda) + (\Delta - 1)(\Delta + \lambda)(1 + \lambda).$

If $n \geq \Delta + 3$, then

$$(n\lambda + n - \Delta\lambda - \Delta + 2\lambda - 2)(2 + \lambda) + (\Delta - 1)(\Delta + \lambda)(1 + \lambda)$$

$$> ((\lambda+1)(n-\Delta) + 2(\lambda-1))(2+\lambda)$$

> $(5\lambda+1)(2+\lambda) + 2(1+\lambda)(2+\lambda) = 7\lambda^2 + 19\lambda + 8 > 0.$

Now, if $n = \Delta + 2$, then $\Delta \ge 4$ and

$$(n\lambda + n - \Delta\lambda - \Delta + 2\lambda - 2)(2 + \lambda) + (\Delta - 1)(\Delta + \lambda)(1 + \lambda)$$

= $((\lambda + 1)(n - \Delta) + 2(\lambda - 1))(2 + \lambda) + (\Delta - 1)(\Delta + \lambda)(1 + \lambda)$
 $\geq 4\lambda^2 + 8\lambda + 3(4 + \lambda)(1 + \lambda) = 7\lambda^2 + 23\lambda + 12 > 0.$

The above computations demonstrate that the lower bound of Theorem 3 is sharper than the lower bound of Theorem A.

Combining Theorems B and 3, we can also state:

Theorem 4. If $\lambda \geq -1$ and Γ is a connected graph of order $n \geq 4$ and maximum degree Δ , then

$$GRM_{\lambda}(\Gamma) \geqslant \begin{cases} (n\lambda + 2n - \Delta\lambda - \Delta - 3)(2 + \lambda) + (\Delta - 1)(\Delta + \lambda)(1 + \lambda); & \Delta < n - 1 \\ \\ \Delta(\Delta + \lambda)(1 + \lambda); & \Delta = n - 1. \end{cases}$$

The equality holds if Γ is a spider with at most one leg of length more than one.

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