Improved Lower Bounds on the General Reduced Second Zagreb Index of Trees and Unicyclic Graphs

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Abstract

For a simple graph Γ and a real number λ, the general reduced second Zagreb index is defined by the formula

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

A sharp lower bound for GRM_λ over all trees of given order and maximum degree under the condition that $\lambda \geq -\frac{1}{2}$ is established. A parallel result is proved for unicyclic graphs under the condition $\lambda \geq -\frac{1}{2}$. The corresponding minimal trees and unicyclic graphs are identified. These findings improve upon the lower bounds previously established by Buyantogtokh, Horoldagva, and Das concerning GRM_λ of trees and unicyclic graphs of given order.

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1 Introduction

Consider a simple graph Γ where $V(\Gamma)$ denotes its vertex set and $E(\Gamma)$ denotes its edge set. For a vertex $a \in V(\Gamma)$, 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, denoted as $\deg_\Gamma(a)$, is given by the order of its open neighborhood. Additionally, the distance between two vertices $a, b \in V(\Gamma)$, defined as the length of any shortest path in Γ that connects a and b, is denoted by $d_\Gamma(a, b)$.

Topological indices are numerical descriptors derived from the molecular graph of a chemical compound, where atoms are represented as vertices and bonds as edges. These indices act as graph invariants, remaining unchanged under structural isomorphisms. They are widely used in chemical graph theory and quantitative structure-activity relationships (QSARs), linking the biological activity or properties of molecules to their chemical structures. Vertex-degree-based topological indices are a specific category of topological indices that evaluate the characteristics of a graph by concentrating on the degrees of its vertices. These indices are defined using a set of real numbers that correspond to pairs of vertex degrees.

The first Zagreb index [16] and the second Zagreb index [15] are foundational members of the family of vertex-degree-based topological indices. These indices are defined for a graph Γ as follows:

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

These indices have significant applications across multiple fields, such as chemistry and network analysis, where they aid in characterizing molecular structures and network topology. For a comprehensive and transparent overview of the Zagreb indices, see Ali et al. [3], Borovićanin et al. [6], and Gutman et al. [14]. However, research in this area remains ongoing, with recent contributions from Ahmad et al. [1], Lin and Qian [20], Pirzada and Khan [24], Täubig [26], Yuan [30], and Das et al. [9] providing new insights and advancements.

Alongside the Zagreb indices, various other vertex-degree-based indices have been proposed. These include the atom-bond connectivity index [11], the sum connectivity index [31], irregularity indices [2, 5], variable Zagreb indices [23, 22], multiplicative Zagreb indices [27, 28], the Lanzhou index [10, 29], and entire Zagreb indices [4, 21].

Furtula et al. [12] demonstrated 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

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

This index has been studied in various contexts, including the works of Li et al. [19], Buyantogtokh et al. [7], Gao and Xu [13], and Shafique and Ali [25].

In 2019, Horoldagva et al. [17] extended the reduced second Zagreb index to the general reduced second Zagreb index $GRM_\lambda(\Gamma)$, 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, fixed real number. This definition can also be expressed equivalently as

$$GRM_\lambda(\Gamma) = M_2(\Gamma) + \lambda M_1(\Gamma) + \lambda^2 |E(\Gamma)|.$$

This general version of the index has garnered considerable interest in recent research [17, 8, 18], reflecting its significance in graph theory and its applications in chemical graph theory. The exploration of $GRM_\lambda(\Gamma)$ not only enhances our understanding of vertex-degree-based indices but also opens new avenues for analyzing the structural properties of graphs.

1.1 Our primary motivation

Our primary motivation for this paper arises from the following two results presented in [8] on the general reduced second Zagreb index of trees and unicyclic graphs.

Theorem A. *If $\lambda \geq -\frac{1}{2}$ and T is a tree with n vertices, then*

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

When $n = 4$ and $\lambda = -\frac{1}{2}$, equality is achieved if and only if $T = P_4$ (a path graph with 4 vertices) or $T = K_{1,3}$ (a star graph with 4 vertices). For all other cases, equality is achieved if and only if $T = P_n$ (a path graph with n vertices).

Theorem B. *If $\lambda \geq -\frac{1}{2}$ and U is a unicyclic graph with n vertices, then*

$$GRM_\lambda(U) \geq n\,(2 + \lambda)^2,$$

where equality holds if and only if $T = C_n$ (a cycle graph with n vertices).

1.2 Our results

In this paper, we extend and refine the bounds established in Theorem A and Theorem B by proving the following two theorems. Denoting by $\mathcal{T}_{n,\Delta}$ the set of all trees with n vertices and a maximum degree of Δ, the first results reads as follows.

Theorem 1. *If $\lambda \geq -\frac{1}{2}$, $n \geq 3$, and $T \in \mathcal{T}_{n,\Delta}$, then*

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

The equality holds if and only if T is a spider graph (a tree with at most one vertex of a degree greater than two) with at most one leg of length more than one.

Let $\mathcal{U}_{n,\Delta}$ denote the set of all unicyclic graphs with n vertices and maximum degree Δ. Let $\mathcal{U}_{n,\Delta}^{(2)}$ be a subset of $\mathcal{U}_{n,\Delta}$ which contains unicyclic graphs U_2 constructed as follows. U_2 is obtained from the disjoint union of a cycle C and a star $K_{1,\Delta-1}$ by adding a path of length at least 2 between the center a of $K_{1,\Delta-1}$ and a vertex b of C, as shown in Fig. 1.

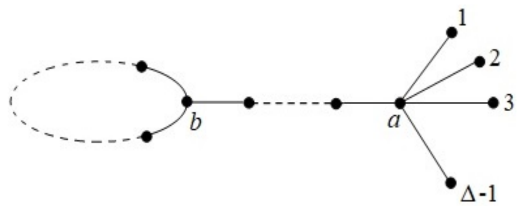

Figure 1: The construction of unicyclic graphs from $\mathcal{U}_{n,\Delta}^{(2)}$.

Let further $U_{n,\Delta}^{(3)}$ be a unicyclic graph from $\mathcal{U}_{n,\Delta}$ obtained by identifying a vertex a of the cycle $C_{n-(\Delta-2)}$ and the center of a star $K_{1,\Delta-2}$, as shown in Fig. 2.

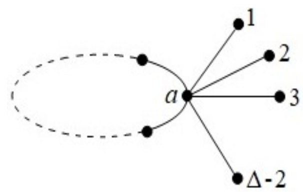

Figure 2: The unicyclic graph $U_{n,\Delta}^{(3)}$.

Our second main result reads as follows.

Theorem 2. *If $\lambda \geq -\frac{1}{2}$, $\Delta \geq 3$, and $U \in \mathcal{U}_{n,\Delta}$, then the following results hold:*

(i) If $2\lambda + 6 < \Delta < n - 3$, then

$$GRM_\lambda(U) \geq (\Delta + \lambda)(\Delta + \Delta\lambda + 1) + (n - \Delta)(2 + \lambda)^2 + 3(2 + \lambda),$$

with equality if and only if $U \in \mathcal{U}_{n,\Delta}^{(2)}$.

(ii) If $3 \leq \Delta < 2\lambda + 6$ or $n - 3 \leq \Delta \leq n - 1$, then

$$GRM_\lambda(U) \geq (\Delta + \lambda)(\Delta + \Delta\lambda + 2) + (n - \Delta)(2 + \lambda)^2,$$

with equality if and only if $U = U_{n,\Delta}^{(3)}$.

(iii) If $\Delta = 2\lambda + 6$, then

$$GRM_\lambda(U) \geq 6(2 + \lambda)^3 + (n - 2\lambda - 6)(2 + \lambda)^2,$$

with equality if and only if either $U \in \mathcal{U}_{n,\Delta}^{(2)}$ or $U = U_{n,\Delta}^{(3)}$.

2 Proof of Theorem 1

In this section we prove Theorem 1 and at the end of the section compare the bounds given in the theorem with those in Theorem A.

A rooted tree is a tree in which one vertex is designated as the root. In this structure, every other vertex is connected to the root either directly or through a sequence of edges, creating a hierarchical organization among the vertices. A *spider* is a specific type of tree that has at most one vertex with a degree greater than two, known as the center of the spider. Each path extending from this center to a leaf vertex (vertex of degree one) is called a *leg*. A *star* is a special case of a spider where all legs have a length of one. By convention, a path graph can also be considered a spider, particularly when it is viewed as having either one leg (a single path) or two legs (two paths extending from a common vertex).

The key lemma for establishing the announced inequality on trees reads as follows.

Lemma 3. *Let $\lambda \geq -\frac{1}{2}$ and $\Delta \geq 3$. If $T \in \mathcal{T}_{n,\Delta}$ contains two distinct vertices a and b such that $\deg_T(a) = \Delta$ and $\deg_T(b) \geq 3$, then there exists $T^* \in \mathcal{T}_{n,\Delta}$ such that $GRM_\lambda(T^*) < GRM_\lambda(T)$.*

Proof. Let T be a rooted tree with root vertex a. Without loss of generality, assume b is the vertex farthest from a among all non root vertices x (i.e., $x \neq a$) satisfying $\deg_T(x) \geq 3$. Let $\deg_T(b) = \ell$, and denote the neighborhood of b as $N_T(b) = \{b_1, b_2, \ldots, b_\ell\}$, where b_ℓ is the unique neighbor of b lying on the path from b to a in T. By our assumption about the maximality of $d_T(a, b)$, every vertex b_i (for $1 \leq i \leq \ell - 1$) satisfies $\deg_T(b_i) \in \{1, 2\}$. These degree constraints lead to three distinct cases:

Case 1: b has at least two leaf neighbors.
Assume without loss of generality that the vertices b_1 and b_2 are two leaves adjacent to b. We construct a modified tree T^* by removing the edge bb_1 and adding the edge b_1b_2. In T^*, vertex b_2 becomes the support vertex for leaf b_1 (see Fig. 3).

We now analyze how this modification affects the general reduced second Zagreb index. Recall that $\lambda \geq -\frac{1}{2}$ and $\ell \geq 3$. We define $X = GRM_\lambda(T) - GRM_\lambda(T^*)$ and calculate it as follows:

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

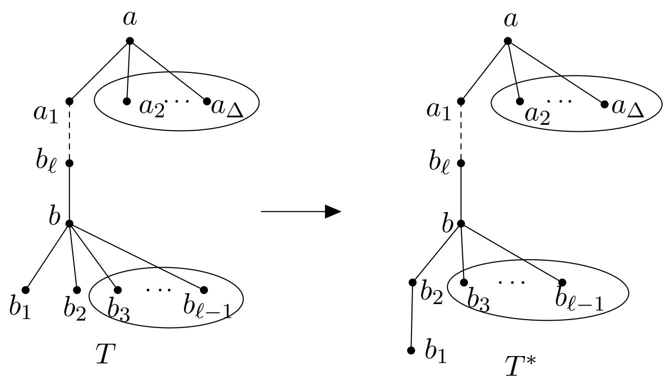

Figure 3: Transformation from Case 1 of Lemma 3.

$$
\begin{aligned}
&+ \sum_{i=3}^{\ell-1} (\ell+\lambda)(\deg_T(b_i)+\lambda) \\
&- (1+\lambda)(2+\lambda) - (2+\lambda)(\ell-1+\lambda) - (\ell-1+\lambda)(\deg_T(b_\ell)+\lambda) \\
&- \sum_{i=3}^{\ell-1} (\ell-1+\lambda)(\deg_T(b_i)+\lambda) \\
&= \lambda\ell - \lambda + \deg_T(b_\ell) + \sum_{i=3}^{\ell-1}(\deg_T(b_i)+\lambda) \\
&\geq \lambda(\ell-1) + 2 + (1+\lambda)(\ell-3) \\
&= 2\lambda\ell - 4\lambda + \ell - 1 \\
&= 2\lambda(\ell-2) + (\ell-2) + 1 \\
&= (1+2\lambda)(\ell-2) + 1 > 0.
\end{aligned}
$$

Case 2: b has exactly one leaf neighbor.
Let b_1 be the leaf adjacent to b. Consider the path $bc_1c_2\dots c_k$, where $c_1 = b_2$, c_k is a leaf, and $k \geq 2$. Construct a modified tree T^* by removing the leaf b_1, detaching the subpath $c_1c_2\dots c_k$ from b, and attaching the extended path $c_1c_2\dots c_kb_1$ to b. This reorganization creates a new leaf b_1 at the path's terminus (see Fig. 4).

Using the fact that $\lambda \geq -\frac{1}{2}$ and $\ell \geq 3$, and defining $X = GRM_\lambda(T) - GRM_\lambda(T^*)$, we have:

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

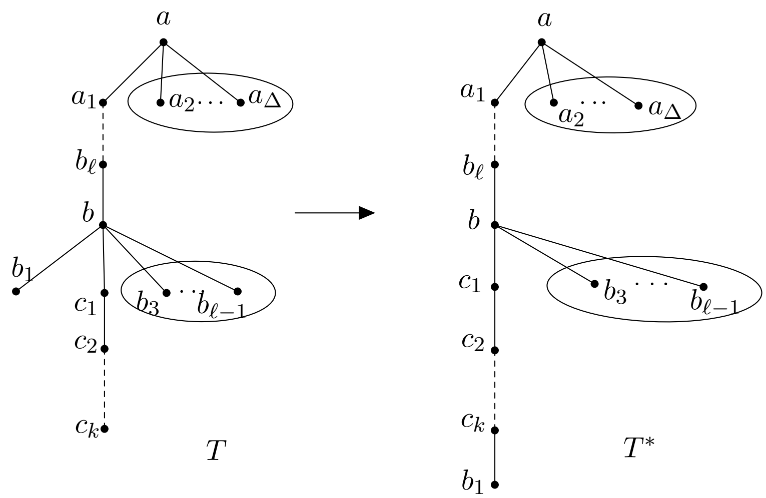

Figure 4: The construction from Case 2 of Lemma 3.

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

Case 3: b has no leaf neighbors.
Consider two paths $bc_1c_2\dots c_k$ and $bd_1d_2\dots d_s$ with $c_1=b_1$ and $d_1=b_2$, where both paths have length at lease two (i.e., $k,s\geq 2$) and terminal nodes c_k and d_s are leaves. Construct a modified tree T^* by detaching the path $c_1c_2\dots c_k$ from b and attaching it to d_s (see Fig. 5).

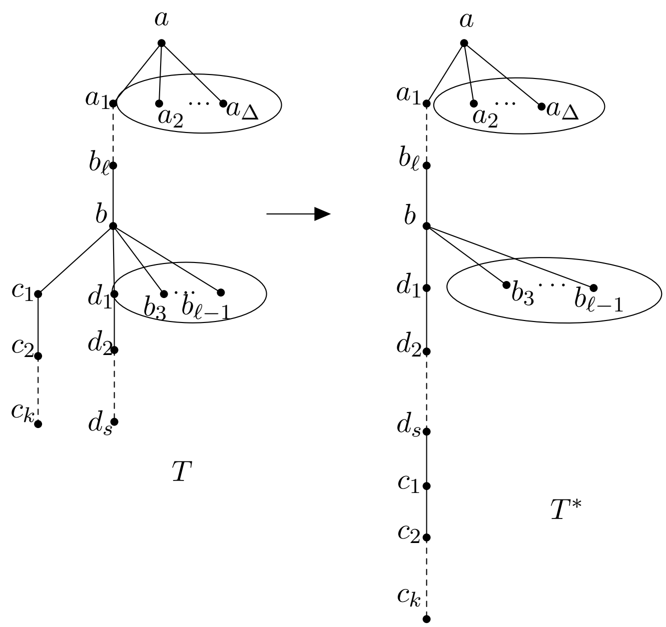

Figure 5: Transformation from Case 3 of Lemma 3.

Once again, let $X = GRM_\lambda(T) - GRM_\lambda(T^*)$. We can estimate it as follows:

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

$$= (2+\lambda)(\ell-3) + \sum_{i=2}^{\ell}(\deg_T(b_i)+\lambda)$$
$$\geq (2+\lambda)(\ell-3) + (2+\lambda)(\ell-1) = 2(2+\lambda)(\ell-2) > 0.$$

This concludes the demonstration of Lemma 3. □

Our second lemma addresses spiders.

Lemma 4. *If T is a spider graph in $\mathcal{T}_{n,\Delta}$ with $\Delta \geq 3$, and it has at least two legs of length greater than one, then there exists another spider graph T^* in $\mathcal{T}_{n,\Delta}$ such that $GRM_\lambda(T^*) < GRM_\lambda(T)$.*

Proof. Let a be the center of T, and consider two legs of length greater than one represented by the paths $ab_1b_2\dots b_t$ and $ac_1c_2\dots c_k$. Construct T^* by detaching the subpath $b_2\dots b_t$ from a and attaching it to the terminal vertex c_k. Define X as $X = GRM_\lambda(T) - GRM_\lambda(T^*)$. Then

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

and we are done. □

We now proceed to establish the proof of Theorem 1.

Let T^* be a tree in $\mathcal{T}_{n,\Delta}$ such that $GRM_\lambda(T^*) \leq GRM_\lambda(T)$ for all T in $\mathcal{T}_{n,\Delta}$. Suppose T^* is rooted at a with $\deg_{T^*}(a) = \Delta$. If $\Delta = 2$, then T^* is a path of order $n \geq 3$, and its general reduced second Zagreb index is given by:

$$GRM_\lambda(T^*) = GRM_\lambda(P_n) = (n-3)(2+\lambda)^2 + 2(1+\lambda)(2+\lambda).$$

Given $\Delta \geq 3$, Lemma 3 ensures that T^* is a spider graph centered at vertex a. Furthermore, Lemma 4 guarantees that T^* has at most one leg of length exceeding one. If all legs of T^* have length one, then T^* is a star, $\Delta = n-1$, and its general reduced second Zagreb index is given by:

$$GRM_\lambda(T^*) = GRM_\lambda(S_n) = (n-1)(n-1+\lambda)(1+\lambda).$$

Assume T^* is not a star and has exactly one leg of length exceeding one. Then $\Delta < n-1$ and we have

$$GRM_\lambda(T^*) = (n-\Delta-2)(2+\lambda)^2 + (\Delta-1)(\Delta+\lambda)(1+\lambda)$$

$$
\begin{aligned}
&+(\Delta+\lambda)(2+\lambda)+(1+\lambda)(2+\lambda)\\
=&n(2+\lambda)^2-3(2+\lambda)+(1+\lambda)(\Delta^2-3\Delta-\lambda),
\end{aligned}
$$

from which the desired result follows.

To end the section, we compare the bounds given in Theorem A and Theorem 1. At first consider the case when $\lambda \geq -\frac{1}{2}$ and $\Delta = n-1$. If $n=3$, then $T = P_3$ and both bounds yield the exact value of $GRM_\lambda(P_3)$ that is $2(1+\lambda)(2+\lambda)$. If $n \geq 4$, then

$$
\begin{aligned}
&(n-1)(n-1+\lambda)(1+\lambda)-(2+\lambda)(n+2\lambda-1)\\
=\ &(n-3)\big(\lambda^2+n(\lambda+1)+(\lambda-1)\big)\\
\geq\ &(4-3)\big(0+4(-\frac{1}{2}+1)-\frac{1}{2}-1\big)=\frac{1}{2}>0.
\end{aligned}
$$

If $\lambda \geq -\frac{1}{2}$ and $\Delta < n-1$, then $n \geq 4$ and we have:

$$
\begin{aligned}
&n(2+\lambda)^2-3(2+\lambda)+(1+\lambda)(\Delta^2-3\Delta-\lambda)-(2+\lambda)(n+2\lambda-1)\\
=\ &(1+\lambda)\big((\Delta-\frac{3}{2})^2+(n-3)\lambda+2n-\frac{25}{4}\big)\\
\geq\ &(-\frac{1}{2}+1)\big((2-\frac{3}{2})^2-\frac{1}{2}(n-3)+2n-\frac{25}{4}\big)\\
=\ &\frac{3}{4}(n-3)>0.
\end{aligned}
$$

The calculations show that the lower bound established in Theorem 1 is stronger than the one presented in Theorem A.

3 Proof of Theorem 2

In this section we prove Theorem 2 and provide a comparison between the bound of our theorem with the bound of Theorem B.

Let $\mathcal{U}_{n,\Delta}$ represent the set of all unicyclic graphs with n vertices and maximum degree Δ. If U is a graph in $\mathcal{U}_{n,2}$, then U must be the cycle graph C_n, for which the general reduced second Zagreb index is given by:

$$GRM_\lambda(U) = n(2+\lambda)^2.$$

For the remainder of this section, we assume $\Delta \geq 3$. To establish the announced inequality for unicyclic graphs, we first need to prove several key lemmas.

Lemma 5. *Assume $\lambda \geq -\frac{1}{2}$, and let U be a unicyclic graph in $\mathcal{U}_{n,\Delta}$, where no vertex of degree Δ lies on the cycle. Suppose $\deg_U(a) = \Delta$, and let b be a vertex on the cycle of U that minimizes the distance $d_U(a,b)$. If either $\deg_U(b) \geq 4$ or there exists a vertex c (distinct from a and b) with $\deg_U(c) \geq 3$, then $\mathcal{U}_{n,\Delta}$ contains another unicyclic graph U' such that $GRM_\lambda(U) > GRM_\lambda(U')$.*

Proof. Let C denote the cycle of U, and let P be the path connecting a to b. Consider a vertex c in U, distinct from a and b, such that $\deg_U(c) \geq 3$. Define T_c as the rooted tree with c as its root, which maximizes the number of vertices connected to c.

If c is not a vertex of the cycle C and the path P, then by Lemma 3, we can transform T_c into a path P_c with the same number of vertices, such that $GRM_\lambda(T_c) > GRM_\lambda(P_c)$. Construct U' in $\mathcal{U}_{n,\Delta}$ by removing T_c from U and replacing it with P_c. Consequently, it follows that $GRM_\lambda(U) > GRM_\lambda(U')$.

Now, let c be a vertex lying either on the cycle C or on the path P. We consider the case where c is a vertex on the cycle C; the case in which c lies on the path P can be proved analogously. Let c_1 and c_2 denote the neighbors of c on C, excluding any vertices that belong to T_c. By Lemma 3, we can transform T_c into a path P_c with the same number of vertices, such that $GRM_\lambda(T_c) \geq GRM_\lambda(P_c)$. Let $P_c = \gamma_1\gamma_2 \cdots \gamma_k$, where $\gamma_1 = c$. Construct the new unicyclic graph U' in $\mathcal{U}_{n,\Delta}$ by removing the rooted tree T_c from U and replacing it with the path P_c. It follows that, $GRM_\lambda(U) \geq GRM_\lambda(U')$ and $\deg_{U'}(c) = 3$. Construct the unicyclic graph $U'' \in \mathcal{U}_{n,\Delta}$ by removing the vertices $\gamma_2, \cdots, \gamma_k$ from U' and replacing the edge cc_1 by the path $c\gamma_2 \cdots \gamma_k c_1$. Consequently, we have:

$$\deg_{U''}(c_1) = \deg_{U'}(c_1) = \deg_U(c_1),$$

$$\deg_{U''}(c_2) = \deg_{U'}(c_2) = \deg_U(c_2).$$

In the subsequent computations we set $X = GRM_\lambda(U') - GRM_\lambda(U'')$.

If the length of P_c is greater than one, then

$$\begin{aligned}
X =\ & (\deg_{U'}(c_1) + \lambda)(\deg_{U'}(c) + \lambda) + (\deg_{U'}(c_2) + \lambda)(\deg_{U'}(c) + \lambda) \\
& + (\deg_{U'}(\gamma_2) + \lambda)(\deg_{U'}(c) + \lambda) + (\deg_{U'}(\gamma_{k-1}) + \lambda)(\deg_{U'}(\gamma_k) + \lambda) \\
& - (\deg_{U''}(c_1) + \lambda)(\deg_{U''}(\gamma_k) + \lambda) - (\deg_{U''}(c_2) + \lambda)(\deg_{U''}(c) + \lambda) \\
& - (\deg_{U''}(\gamma_2) + \lambda)(\deg_{U''}(c) + \lambda) - (\deg_{U''}(\gamma_{k-1}) + \lambda)(\deg_{U''}(\gamma_k) + \lambda) \\
=\ & (\deg_U(c_1) + \lambda)(3 + \lambda) + (\deg_U(c_2) + \lambda)(3 + \lambda) \\
& + (2 + \lambda)(3 + \lambda) + (2 + \lambda)(1 + \lambda) \\
& - (\deg_U(c_1) + \lambda)(2 + \lambda) - (\deg_U(c_2) + \lambda)(2 + \lambda) - 2(2 + \lambda)^2 \\
=\ & \deg_U(c_1) + \deg_U(c_2) + 2\lambda > 0.
\end{aligned}$$

If, however, the length of P_c is one, then

$$\begin{aligned}
X =\ & (\deg_{U'}(c_1) + \lambda)(\deg_{U'}(c) + \lambda) + (\deg_{U'}(c_2) + \lambda)(\deg_{U'}(c) + \lambda) \\
& + (\deg_{U'}(\gamma_2) + \lambda)(\deg_{U'}(c) + \lambda) \\
& - (\deg_{U''}(c_1) + \lambda)(\deg_{U''}(\gamma_2) + \lambda) - (\deg_{U''}(c_2) + \lambda)(\deg_{U''}(c) + \lambda) \\
& - (\deg_{U''}(\gamma_2) + \lambda)(\deg_{U''}(c) + \lambda) \\
=\ & (\deg_U(c_1) + \lambda)(3 + \lambda) + (\deg_U(c_2) + \lambda)(3 + \lambda) + (1 + \lambda)(3 + \lambda) \\
& - (\deg_U(c_1) + \lambda)(2 + \lambda) - (\deg_U(c_2) + \lambda)(2 + \lambda) - (2 + \lambda)^2
\end{aligned}$$

$$= \deg_U(c_1) + \deg_U(c_2) + 2\lambda - 1 > 0.$$

Finally, suppose $\deg_U(b) \geq 4$, with b_1, b_2, and b_3 as neighbors of b in U, where b_1 and b_2 are on the cycle C, and b_3 is on the path P. Define T_b as the rooted tree with the maximum number of vertices connected to b, excluding b_1, b_2, and b_3. By Lemma 3, we can transform T_b into a path P_b with the same number of vertices, such that $GRM_\lambda(T_b) \geq GRM_\lambda(P_b)$. Let $P_b = \beta_1\beta_2\cdots\beta_t$, where $\beta_1 = b$. Construct the new unicyclic graph U' in $\mathcal{U}_{n,\Delta}$ by removing the rooted tree T_b from U and replacing it with the path P_b. It follows that $GRM_\lambda(U) \geq GRM_\lambda(U')$ and $\deg_{U'}(b) = 4$. Construct the unicyclic graph U'' in $\mathcal{U}_{n,\Delta}$ by removing the vertices $\beta_2, \cdots, \beta_t$ from U' and replacing the edge bb_1 with the path $b\beta_2\cdots\beta_t b_1$. Consequently, we have:

$$\deg_{U''}(b_1) = \deg_{U'}(b_1) = \deg_U(b_1),$$
$$\deg_{U''}(b_2) = \deg_{U'}(b_2) = \deg_U(b_2),$$
$$\deg_{U''}(b_3) = \deg_{U'}(b_3) = \deg_U(b_3).$$

If the length of P_b is at least two, then

$$\begin{aligned}
X = &(\deg_{U'}(b_1) + \lambda)(\deg_{U'}(b) + \lambda) + (\deg_{U'}(b_2) + \lambda)(\deg_{U'}(b) + \lambda)\\
&+ (\deg_{U'}(b_3) + \lambda)(\deg_{U'}(b) + \lambda) + (\deg_{U'}(\beta_2) + \lambda)(\deg_{U'}(b) + \lambda)\\
&+ (\deg_{U'}(\beta_{t-1}) + \lambda)(\deg_{U'}(\beta_t) + \lambda)\\
&- (\deg_{U''}(b_1) + \lambda)(\deg_{U''}(\beta_t) + \lambda) - (\deg_{U''}(b_2) + \lambda)(\deg_{U''}(b) + \lambda)\\
&- (\deg_{U''}(b_3) + \lambda)(\deg_{U''}(b) + \lambda) - (\deg_{U''}(\beta_2) + \lambda)(\deg_{U''}(b) + \lambda)\\
&- (\deg_{U''}(\beta_{t-1}) + \lambda)(\deg_{U''}(\beta_t) + \lambda)\\
= &(\deg_U(b_1) + \lambda)(4 + \lambda) + (\deg_U(b_2) + \lambda)(4 + \lambda)\\
&+ (\deg_U(b_3) + \lambda)(4 + \lambda) + (2 + \lambda)(4 + \lambda) + (2 + \lambda)(1 + \lambda)\\
&- (\deg_U(b_1) + \lambda)(2 + \lambda) - (\deg_U(b_2) + \lambda)(3 + \lambda)\\
&- (\deg_U(b_3) + \lambda)(3 + \lambda) - (2 + \lambda)(3 + \lambda) - (2 + \lambda)^2\\
= &2\deg_U(b_1) + \deg_U(b_2) + \deg_U(b_3) + 4\lambda > 0.
\end{aligned}$$

If, however, the length of P_b is one, then

$$\begin{aligned}
X = &(\deg_{U'}(b_1) + \lambda)(\deg_{U'}(b) + \lambda) + (\deg_{U'}(b_2) + \lambda)(\deg_{U'}(b) + \lambda)\\
&+ (\deg_{U'}(b_3) + \lambda)(\deg_{U'}(b) + \lambda) + (\deg_{U'}(\beta_2) + \lambda)(\deg_{U'}(b) + \lambda)\\
&- (\deg_{U''}(b_1) + \lambda)(\deg_{U''}(\beta_2) + \lambda) - (\deg_{U''}(b_2) + \lambda)(\deg_{U''}(b) + \lambda)\\
&- (\deg_{U''}(b_3) + \lambda)(\deg_{U''}(b) + \lambda) - (\deg_{U''}(\beta_2) + \lambda)(\deg_{U''}(b) + \lambda)\\
= &(\deg_U(b_1) + \lambda)(4 + \lambda) + (\deg_U(b_2) + \lambda)(4 + \lambda)\\
&+ (\deg_U(b_3) + \lambda)(4 + \lambda) + (1 + \lambda)(4 + \lambda)\\
&- (\deg_U(b_1) + \lambda)(2 + \lambda) - (\deg_U(b_2) + \lambda)(3 + \lambda)\\
&- (\deg_U(b_3) + \lambda)(3 + \lambda) - (2 + \lambda)(3 + \lambda)
\end{aligned}$$

$$= 2\deg_U(b_1) + \deg_U(b_2) + \deg_U(b_3) + 4\lambda - 2 > 0.$$

This concludes the proof of Lemma 5. □

As the proof of the next lemma closely resembles the one presented in Lemma 5, it is omitted for brevity.

Lemma 6. *Assuming $\lambda \geq -\frac{1}{2}$, consider a graph U in $\mathcal{U}_{n,\Delta}$ with a vertex a of degree Δ on its cycle. If U contains another vertex b (excluding a) of a degree of at least 3, then there exists a unicyclic graph U' in $\mathcal{U}_{n,\Delta}$ where $GRM_\lambda(U) > GRM_\lambda(U')$.*

Lemma 7. *Let $\lambda \geq -\frac{1}{2}$ and let $U \in \mathcal{U}_{n,\Delta}$ have the vertex a of degree Δ that is not on its cycle. If a is adjacent to at least two vertices of degree more than one, then $\mathcal{U}_{n,\Delta}$ contains a unicyclic graph U' such that $GRM_\lambda(U) > GRM_\lambda(U')$.*

Proof. Let b be a vertex on the cycle of U minimizing the distance $d_U(a, b)$ and let P be the unique path connecting a and b. Assume that T_a is the tree rooted at a with the maximum possible number of vertices that are connected to a by paths, and it satisfies $deg_{T_a}(a) = \Delta - 1$ and $V(T_a) \cap V(P) = \{a\}$. According to the transformations described in Lemma 3, we can transform the tree T_a into a spider tree T'_a with the same number of vertices, the same root a, and $\Delta - 1$ legs, such that $V(T'_a) \cap V(P) = \{a\}$ and $GRM_\lambda(T_a) \geq GRM_\lambda(T'_a)$. Now, consider the unicyclic graph U' in $\mathcal{U}_{n,\Delta}$ obtained by replacing T_a with T'_a. Consequently, it holds that $GRM_\lambda(U) \geq GRM_\lambda(U')$.

Suppose a is adjacent to at least two vertices of degree greater than one. By Theorem 1, T'_a takes the form of a spider graph with one leg longer than one, such as $P' = c_1\, c_2\, \ldots c_k$. Let c_1 be a vertex in $N_{U'}(a) \cap V(P')$, and select $d \in N_{U'}(a) \setminus \{c_1\}$ so that d is on the path P. Now, derive a new unicyclic graph U'' in $\mathcal{U}_{n,\Delta}$ by removing $c_2, \ldots, c_k$ from U' and adding the path $d\, c_2\, \ldots c_k\, a$. According to Lemma 5, we can assume that $\deg_{U''}(d) = \deg_{U'}(d) = 2$ when $d \neq b$ and $\deg_{U''}(d) = \deg_{U'}(d) = 3$ when $d = b$. If $\deg_{U''}(d) = \deg_{U'}(d) = 2$, then recalling that $X = GRM_\lambda(U') - GRM_\lambda(U'')$, we have

$$\begin{aligned} X &= 2(2+\lambda)(\Delta+\lambda) + (2+\lambda)(1+\lambda) \\ &\quad - (2+\lambda)(\Delta+\lambda) - (1+\lambda)(\Delta+\lambda) - (2+\lambda)(2+\lambda) \\ &= \Delta - 2 > 0, \end{aligned}$$

and if $\deg_{U''}(d) = \deg_{U'}(d) = 3$, then

$$\begin{aligned} X &= (3+\lambda)(\Delta+\lambda) + (2+\lambda)(\Delta+\lambda) + (2+\lambda)(1+\lambda) \\ &\quad - (2+\lambda)(\Delta+\lambda) - (1+\lambda)(\Delta+\lambda) - (3+\lambda)(2+\lambda) \\ &= 2\Delta - 4 > 0, \end{aligned}$$

which proves Lemma 7. □

The proof of the next lemma closely resembles the one presented in Lemma 7, so it will be omitted.

Lemma 8. *Let $\lambda \geq -\frac{1}{2}$ and let $U \in \mathcal{U}_{n,\Delta}$ have the vertex a of degree Δ on its cycle. If a is adjacent to at least three vertices of degree greater than one, then $\mathcal{U}_{n,\Delta}$ contains a unicyclic graph U' such that $GRM_\lambda(U) > GRM_\lambda(U')$.*

From Lemmas 5–8, we verify that within the set $\mathcal{U}_{n,\Delta}$, the minimal unicyclic graphs with respect to GRM_λ must either belong to the subset $\mathcal{U}^{(2)}_{n,\Delta}$, or coincide with one of the graphs $U^{(1)}_{n,\Delta}$ or $U^{(3)}_{n,\Delta}$. These structures are formally defined as follows:

- Let $U^{(1)}_{n,\Delta}$ be a unicyclic graph from $\mathcal{U}_{n,\Delta}$ with a vertex a of degree Δ, where a is adjacent to $\Delta - 1$ leaves and a is not on the cycle of $U^{(1)}_{n,\Delta}$. Additionally, let b be a vertex on the cycle of $U^{(1)}_{n,\Delta}$ such that $d_{U^{(1)}_{n,\Delta}}(a,b) = 1$, $\deg_{U^{(1)}_{n,\Delta}}(b) = 3$, and for every vertex $c \in V(U^{(1)}_{n,\Delta}) \setminus \{a,b\}$, it holds that $1 \leq \deg_{U^{(1)}_{n,\Delta}}(c) \leq 2$ (see Fig. 6). Then

$$\begin{aligned} GRM_\lambda(U^{(1)}_{n,\Delta}) =& 2(3+\lambda)(2+\lambda) + (\Delta-1)(1+\lambda)(\Delta+\lambda) + (3+\lambda)(\Delta+\lambda) \\ &+ (n-\Delta-2)(2+\lambda)^2 \\ =& (\Delta+\lambda)(\Delta+\Delta\lambda+2) + (n-\Delta)(2+\lambda)^2 + 2(2+\lambda). \end{aligned} \quad (1)$$

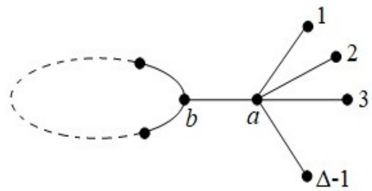

Figure 6: The unicyclic graph $U^{(1)}_{n,\Delta}$.

- Let $\mathcal{U}^{(2)}_{n,\Delta}$ be a subset of $\mathcal{U}_{n,\Delta}$ such that every unicyclic graph $U_2 \in \mathcal{U}^{(2)}_{n,\Delta}$ has a vertex a of degree Δ, where a is adjacent to $\Delta-1$ leaves and is not part of the cycle. Additionally, assume b is a vertex on the cycle of U_2 such that the distance $d_{U_2}(a,b)$ is minimized, specifically with $d_{U_2}(a,b) \geq 2$, $\deg_{U_2}(b) = 3$, and for every vertex $c \in V(U_2) \setminus \{a,b\}$, it holds that $1 \leq \deg_{U_2}(c) \leq 2$ (see Fig. 1). Therefore, for every unicyclic graph $U_2 \in \mathcal{U}^{(2)}_{n,\Delta}$, we have

$$\begin{aligned} GRM_\lambda(U_2) =& 3(3+\lambda)(2+\lambda) + (\Delta-1)(1+\lambda)(\Delta+\lambda) + (2+\lambda)(\Delta+\lambda) \\ &+ (n-\Delta-3)(2+\lambda)^2 \\ =& (\Delta+\lambda)(\Delta+\Delta\lambda+1) + (n-\Delta)(2+\lambda)^2 + 3(2+\lambda). \end{aligned} \quad (2)$$

- Let $U^{(3)}_{n,\Delta}$ be a unicyclic graph from $\mathcal{U}_{n,\Delta}$ with a vertex a on its cycle, where a has degree Δ and is adjacent to $\Delta-2$ leaves. Additionally, for every vertex $b \in V(U^{(3)}_{n,\Delta}) \setminus \{a\}$, it holds that $1 \leq \deg_{U^{(3)}_{n,\Delta}}(b) \leq 2$ (see Fig. 2). Then

$$\begin{aligned} GRM_\lambda(U^{(3)}_{n,\Delta}) =&(\Delta-2)(1+\lambda)(\Delta+\lambda)+2(2+\lambda)(\Delta+\lambda)+(n-\Delta)(2+\lambda)^2 \\ =&(\Delta+\lambda)(\Delta+\Delta\lambda+2)+(n-\Delta)(2+\lambda)^2. \end{aligned} \tag{3}$$

Now, we compare GRM_λ values across these subsets.

Lemma 9. *For each unicyclic graph $U_2 \in \mathcal{U}^{(2)}_{n,\Delta}$, we have*

$$GRM_\lambda(U^{(1)}_{n,\Delta}) > GRM_\lambda(U_2).$$

Proof. By subtracting Eq. (2) from Eq. (1), we obtain

$$GRM_\lambda(U^{(1)}_{n,\Delta}) - GRM_\lambda(U_2) = \Delta - 2 > 0,$$

from which the result follows. □

Lemma 10. *The following inequality holds:*

$$GRM_\lambda(U^{(1)}_{n,\Delta}) > GRM_\lambda(U^{(3)}_{n,\Delta}).$$

Proof. By subtracting Eq. (3) from Eq. (1), we obtain

$$GRM_\lambda(U^{(1)}_{n,\Delta}) - GRM_\lambda(U^{(3)}_{n,\Delta}) = 2(2+\lambda) > 0,$$

from which the result follows. □

Lemma 11. *For each unicyclic graph $U_2 \in \mathcal{U}^{(2)}_{n,\Delta}$, the following inequalities hold:*

If $\Delta > 2\lambda + 6$, then $GRM_\lambda(U^{(3)}_{n,\Delta}) > GRM_\lambda(U_2)$.

If $\Delta < 2\lambda + 6$, then $GRM_\lambda(U_2) > GRM_\lambda(U^{(3)}_{n,\Delta})$.

If $\Delta = 2\lambda + 6$, then $GRM_\lambda(U^{(3)}_{n,\Delta}) = GRM_\lambda(U_2)$.

Proof. By subtracting Eq. (2) from Eq. (3), we obtain:

$$GRM_\lambda(U^{(3)}_{n,\Delta}) - GRM_\lambda(U_2) = \Delta - 2\lambda - 6.$$

It can now be easily verified that, if $\Delta > 2\lambda + 6$, then $GRM_\lambda(U^{(3)}_{n,\Delta}) > GRM_\lambda(U_2)$, if $\Delta < 2\lambda + 6$, then $GRM_\lambda(U_2) > GRM_\lambda(U^{(3)}_{n,\Delta})$, and if $\Delta = 2\lambda + 6$, then $GRM_\lambda(U^{(3)}_{n,\Delta}) = GRM_\lambda(U_2)$. □

With all the prerequisites in place, we can now proceed to establish the proof of Theorem 2.

Assume that $U' \in \mathcal{U}_{n,\Delta}$ with $GRM_\lambda(U) \geq GRM_\lambda(U')$ for every $U \in \mathcal{U}_{n,\Delta}$. By Lemmas 5–11, U' satisfies one of the following cases:

Case 1. If $2\lambda + 6 < \Delta < n - 3$, then $U' \in \mathcal{U}^{(2)}_{n,\Delta}$, and from Eq. (2), we obtain:

$$GRM_\lambda(U') = (\Delta + \lambda)(\Delta + \Delta\lambda + 1) + (n - \Delta)(2 + \lambda)^2 + 3(2 + \lambda).$$

So the inequality in Theorem 2 (i) holds with equality if and only if $U \in \mathcal{U}^{(2)}_{n,\Delta}$.

Case 2. If $3 \leq \Delta < 2\lambda + 6$ or $n - 3 \leq \Delta \leq n - 1$, then $U' = U^{(3)}_{n,\Delta}$, and from Eq. (3), we have:

$$GRM_\lambda(U') = (\Delta + \lambda)(\Delta + \Delta\lambda + 2) + (n - \Delta)(2 + \lambda)^2.$$

Hence the inequality in Theorem 2 (ii) holds with equality if and only if $U = U^{(3)}_{n,\Delta}$.

Case 3. If $\Delta = 2\lambda + 6$, then $U' \in \mathcal{U}^{(2)}_{n,\Delta}$ or $U' = U^{(3)}_{n,\Delta}$, and from Eq. (2) or Eq. (3), we get:

$$GRM_\lambda(U') = 6(2 + \lambda)^3 + (n - 2\lambda - 6)(2 + \lambda)^2.$$

Then the inequality in Theorem 2 (iii) holds with equality if and only if either $U \in \mathcal{U}^{(2)}_{n,\Delta}$ or $U = U^{(3)}_{n,\Delta}$. This completes the proof of Theorem 2.

We end this section with providing a comparison between the bound of Theorem B and that of Theorem 2.

If $2\lambda + 6 < \Delta < n - 3$, then

$$\begin{aligned}&(\Delta + \lambda)(\Delta + \Delta\lambda + 1) + (n - \Delta)(2 + \lambda)^2 + 3(2 + \lambda) - n(2 + \lambda)^2 \\ =\ &(1 + \lambda)(\Delta^2 - 3\Delta + 4) + 2 > 0.\end{aligned}$$

If $3 \leq \Delta \leq 2\lambda + 6$ or $n - 3 \leq \Delta \leq n - 1$, then

$$\begin{aligned}&(\Delta + \lambda)(\Delta + \Delta\lambda + 2) + (n - \Delta)(2 + \lambda)^2 - n(2 + \lambda)^2 \\ =\ &(1 + \lambda)(\Delta^2 - 3) + 2\lambda + \Delta > 0.\end{aligned}$$

The above comparison shows that the lower bound of Theorem 2 is stronger than that of Theorem B, where $\lambda \geq -\frac{1}{2}$.

4 Concluding remarks

In this paper, we have extended and refined the bounds established in Theorem A and Theorem B by deriving sharp lower bounds for the general reduced second Zagreb index of trees and unicyclic graphs with a specified order and maximum degree. Furthermore, we recall the following result.

Theorem C. [17] *If* Γ *is a connected graph and* $\lambda \geq -\frac{1}{2}$, *then for every* $e \notin E(\Gamma)$,

$$GRM_\lambda(\Gamma + e) > GRM_\lambda(\Gamma).$$

This result thus asserts that adding an edge to a connected graph increases the value of the general reduced second Zagreb index. By combining Theorem C with Theorem 1, we can formulate the following additional result.

Theorem 12. *If* $\lambda \geq -\frac{1}{2}$ *and* Γ *is a connected graph of order* $n \geq 3$ *and maximum degree* Δ, *then*

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

The equality condition is met if and only if the graph Γ *is a spider graph with at most one leg of length exceeding one.*

We have also identified the minimal trees and unicyclic graphs that achieve these lower bounds in our main two theorems. The identification of minimal trees and unicyclic graphs provides a framework for future research and applications in mathematical chemistry and network theory. Future research may explore further generalizations of our findings, as well as their implications for other classes of graphs. Additionally, investigating the behavior of the general reduced second Zagreb index under various graph operations could yield new avenues for understanding the structural properties of graphs.

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Author Contributions

All authors contributed equally to the conception, design, investigation, methodology, validation, resources, and writing of this manuscript. All authors have read and approved the final version of the manuscript.

Availability of data and materials

The paper includes or uses no datasets.

Conflicts of Interest

The authors declare that they have no conflict of interest.

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