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Transactions on Combinatorics

ISSN (print): 2251-8657, ISSN (on-line): 2251-8665

Vol. xx No. x (202x), pp. xx-xx.

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BOUNDING THE FIRST ZAGREB INDEX OF A UNICYCLIC GRAPH IN TERM OF ITS REPETITION NUMBER

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ABSTRACT. The first Zagreb index M_1 is equal to the sum of the squares of the degrees of the vertices. The repetition number of a graph is the maximum multiplicity in the list of its vertex degrees. In this paper, we lower and upper bound the first Zagreb index of a unicyclic graph by expressions depending solely on their repetition number and give degree sequence for these graphs with the largest and smallest first Zagreb indices, respectively.

1. Introduction

Throughout this paper, we consider graphs without loops, but they may have multiple edges. Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. A *neighbour* of a vertex u is a vertex adjacent to u . The set of all neighbours of u is denoted by $N_G(u)$. The *degree* of u is defined to be $d_G(u) = |N_G(u)|$. The maximum and minimum degrees of G are denoted by $\Delta = \Delta(G)$ and $\delta = \delta(G)$. The degree sequence of a graph is the list of vertex degrees, usually written in non-increasing order.

The *first Zagreb index* $M_1(G)$ of a graph G is denoted as

$$M_1(G) = \sum_{u \in V(G)} d_G^2(u).$$

MSC(2010): Primary: 05C05; Secondary: 05C07.

Keywords: first Zagreb index, repetition number, unicyclic graph, degree sequence.

Manuscript Type: Research Paper.

Communicated by Bijan Taeri.

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Received: 29 August 2025, Accepted: 25 October 2026, Published Online: dd mmmm yyyy.

Cite this article: M. Wang and R. Liu, Bounding the first Zagreb index of a unicyclic graph in term of its repetition number,

Trans. Comb., x no. x (202x) xx-xx. <https://dx.doi.org/10.22108/toc.2026.146502.2321>.

The first Zagreb index is a widely studied degree-based topological index which was introduced by Gutman and Trinajstić [7] in 1972 and elaborated in [8]. Gutman and Goubko summarized the main mathematical properties of M_1 in the survey [9]. For more results on this topic, we refer the readers the papers [2, 4, 5, 6, 10, 11, 12, 14] and the recent survey [1]

Let n be a positive integer. A sequence of positive integers $(n_1, n_2, \dots, n_k)$ with $n_1 \geq n_2 \geq \dots \geq n_k \geq 1$ is said to be a *partition* of n if $n = n_1 + n_2 + \dots + n_k$. The set of all partitions of n is denoted by $\mathcal{P}_n$. For a positive integer n , we define a function $f(n)$ as follows:

$$f(n) = \max\{(n_1 + 2)^2 + (n_2 + 2)^2 + \dots + (n_k + 2)^2 \mid 1 \leq k \leq n, (n_1, n_2, \dots, n_k) \in \mathcal{P}_n\}.$$

Motivated by the fact that every graph (with no loops or multiedges) has two vertices with the same degree, Caro and West [3] defined the *repetition number* $\text{rep}(G)$ of a graph G to be the maximum multiplicity in the list of its vertex degrees. Generally speaking, the repetition number provides a measure of regularity of a simple graph. For an n -vertex graph G , the largest possible value of $\text{rep}(G)$ is n . If $\text{rep}(G)=n$, then G is a regular graph.

For a connected graph G , the value $c(G) = |E(G)| - |V(G)| + 1$ is called the *cyclomatic number* of G . When $c(G) = 0, 1, 2$, the graph is called a *tree*, a *unicyclic graph* and a *bicyclic graph*. The *cycle* and *path* with n vertices are denoted by C_n and P_n , respectively. The *girth* of a graph is the length of its shortest cycle. We use $\mathbb{T}_r$ (resp., $\mathbb{U}_r$) to denote the set of trees (resp., unicyclic) graphs with repetition number r . Let $r_i(G)$ denote the number of vertices of G with degree i , where $1 \leq i \leq \Delta(G)$.

The following results is obtained in [13].

Theorem 1.1. [13] *Let $T \in \mathbb{T}_r$, where $r \geq 4$. Then*

$$4r + 2 \leq M_1(T) \leq f(r - 2) + 5r.$$

The lower bound is achieved if and only if $T = P_{r+2}$, and if T^* is a tree satisfying the upper bound, then $r_1(T^*) = r_2(T^*) = \text{rep}(T^*)$.

In the same paper, Lin and Qian posed the following Question.

Question 1. [13]. Could such type results as stated in Theorem 1.1 be extended to some classes of graphs with more cycles, such as unicyclic graphs and bicyclic graphs?

In this paper, we focus on the unicyclic graphs and obtain the following result.

Theorem 1.2. *Let G be a unicyclic graph with girth at least 3. If $G \in \mathbb{U}_r$, where $r \geq 5$, then*

$$4r \leq M_1(G) \leq f(r) + 5r.$$

The lower bound is achieved if and only if $G = C_r$, and if G^* is a unicyclic graph satisfying the upper bound, then G^* has degree sequence

$$(r + 2, \underbrace{2, \dots, 2}_r, \underbrace{1, \dots, 1}_r).$$

The paper is organized as follows. In Section 2, we state some preliminary results. In Section 3, we prove Theorem 1.2, and in Section 4, we conclude the work with some concluding remarks.

2. Preliminaries

In a graph, a vertex of degree one is called a *pendent vertex*. A tree is called a *caterpillar* if the removal of all pendent vertices results in a path. For a subgraph H (or a subset of edges) of a graph G , we denote by $G - H$ the subgraph of G obtained by removing the edges in H , that is $V(G - H) = V(G)$ and $E(G - H) = E(G) \setminus E(H)$.

Lemma 2.1. *For any unicyclic graph G , $\text{rep}(G) = \max\{r_1(G), r_2(G)\}$.*

Proof. Suppose to the contrary that $\text{rep}(G) = r_i(G) > \max\{r_1(G), r_2(G)\}$ for some $3 \leq i \leq \Delta(G)$. Set $\Delta(G) = \Delta$ and $r_t = r_t(G)$ for each $1 \leq t \leq \Delta$. Assume that G has n vertices (and thus with n edges). Then

$$(2.1) \quad r_1 + r_2 + \cdots + r_\Delta = n.$$

By the handshaking lemma,

$$(2.2) \quad r_1 + 2r_2 + \cdots + \Delta r_\Delta = 2|E(G)| = 2n.$$

By (2.1) and (2.2), we have

$$\begin{aligned} 2n &= r_1 + 2r_2 + \cdots + \Delta r_\Delta \\ &\geq 2(r_1 + r_2 + r_3 + \cdots + r_{i-1} + r_i + r_{i+1} + \cdots + r_\Delta) + (r_i - r_1) \\ &= 2n + (r_i - r_1) \\ &> 2n, \end{aligned}$$

a contradiction. This completes the proof of Lemma 2.1. □

Lemma 2.2. *Let n be a positive integer. If $n \geq 5$, then $f(n) = (n + 2)^2$.*

Proof. Recall that

$$f(n) = \max \left\{ (n_1 + 2)^2 + (n_2 + 2)^2 + \cdots + (n_k + 2)^2 \mid 1 \leq k \leq n, (n_1, n_2, \dots, n_k) \in \mathcal{P}_n \right\}.$$

If $k = 1$, then we are done. Thus, we assume that $k \geq 2$. Since $n = n_1 + n_2 + \cdots + n_k$,

$$\begin{aligned} (n + 2)^2 &= (n_1 + n_2 + \cdots + n_k + 2)^2 \\ &= (n_1 + n_2 + \cdots + n_k)^2 + 4n + 4 \\ &= \sum_{i=1}^k n_i^2 + 2 \sum_{1 \leq i < j \leq k} n_i n_j + 4n + 4. \end{aligned}$$

On the other hand,

$$(n_1 + 2)^2 + (n_2 + 2)^2 + \cdots + (n_k + 2)^2 = \sum_{i=1}^k n_i^2 + 4n + 4k.$$

Therefore,

$$D := (n + 2)^2 - [(n_1 + 2)^2 + (n_2 + 2)^2 + \cdots + (n_k + 2)^2] = 2 \sum_{1 \leq i < j \leq k} n_i n_j - 4(k - 1).$$

Since $(n_1, n_2, \dots, n_k) \in \mathcal{P}_n$, we have $n_1 \geq n_2 \geq \cdots \geq n_k \geq 1$. We claim that $D > 0$. It suffices to show that

$$\sum_{1 \leq i < j \leq k} n_i n_j > 2(k - 1).$$

Since $n \geq 5$, exactly one of the following three cases occurs:

(1) $n_1 \geq 3$. Then

$$\sum_{1 \leq i < j \leq k} n_i n_j \geq n_1 \sum_{i=2}^k n_i \geq 3(k - 1) > 2(k - 1).$$

(2) $n_1 = 2$ and $k \geq 3$. Let t be the number of parts equal to 2. Then $t \geq 1$, and the remaining $k - t$ parts are equal to 1. Hence

$$\begin{aligned} \sum_{1 \leq i < j \leq k} n_i n_j &= 4 \binom{t}{2} + 2t(k - t) + \binom{k - t}{2} \\ &= 2t(t - 1) + 2t(k - t) + \binom{k - t}{2} \\ &= 2t(k - 1) + \binom{k - t}{2} \end{aligned}$$

If $k - t \geq 2$, then $\binom{k - t}{2} > 0$ and $2t(k - 1) \geq 2(k - 1)$, so

$$\sum_{1 \leq i < j \leq k} n_i n_j > 2(k - 1).$$

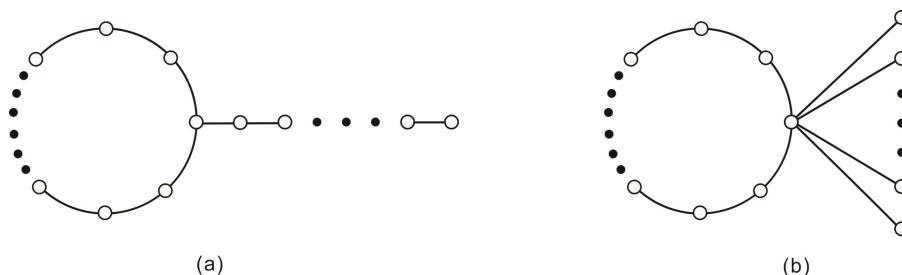
If $k - t \leq 1$, then $t \geq k - 1 \geq 2$, and therefore

$$\sum_{1 \leq i < j \leq k} n_i n_j \geq 2t(k - 1) \geq 4(k - 1) > 2(k - 1).$$

(3) $n_1 = 1$ and $k \geq 5$. Then all $n_i = 1$, so

$$\sum_{1 \leq i < j \leq k} n_i n_j = \binom{k}{2} = \frac{k(k - 1)}{2} > 2(k - 1),$$

since $k \geq 5$ implies $k/2 > 2$.

FIGURE 1. (a) Unicyclic graph F_n^k , (b) Unicyclic graph S_n^k .

Thus in all cases $D = 2 \sum_{i < j} n_i n_j - 4(k-1) > 0$, which means

$$(n_1 + 2)^2 + (n_2 + 2)^2 + \cdots + (n_k + 2)^2 < (n + 2)^2.$$

Therefore the maximum in the definition of $f(n)$ is attained when $k = 1$, i.e., $f(n) = (n + 2)^2$. This completes the proof of Lemma 2.2. $\square$

3. Proof of Theorem 1.2

Let F_n^k be the unicyclic graph obtained by identifying one pendent vertex of P_{n-k+1} with a vertex of C_k , see Figure 1(a). Let S_n^k be the unicyclic graph obtained from the cycle C_k by attaching $n - k$ pendent edges to the same vertex on C_k , see Figure 1(b).

The following theorem, obtained by Deng [4], is an important result on the first Zagreb index of unicyclic graphs.

Theorem 3.1. [4] *Let G be a unicyclic graph of order n and girth $k \geq 3$. If G is different from F_n^k and S_n^k , then*

$$4n \leq M_1(F_n^k) < M_1(G) < M_1(S_n^k) \leq n^2 - n + 6.$$

The lower bound is achieved if and only if $G = C_n = F_n^n$ and the upper bound is attained if and only if $G = S_n^3$.

Proof of Theorem 1.2: Set $|V(G)| = n$. Since $G \in \mathbb{U}_r$ and $r \geq 5$, $n \geq r \geq 5$. If $n = r$, by Lemma 2.1, then G has exactly $n = r$ vertices with same degree one or two. Hence $G = C_r$.

If $n = r + 1$, by Lemma 2.1, then G has exactly $n - 1$ vertices with same degree one or two. However, it is impossible.

If $n \geq r + 2$, note that $F_{r+2}^k \in \mathbb{U}_r$ ($3 \leq k \leq r + 1$), by Theorem 3.1, then

$$M_1(G) \geq M_1(F_{r+2}^k) = 4r + 10,$$

with equality if and only if $n = r + 2$ and $G = F_{r+2}^k$.

It is not hard to calculate that $M_1(C_r) = 4r$. So C_r is the unique graph in $\mathbb{U}_r$ that attains the minimal value of the first Zagreb index.

Now we turn to determine the upper bound of $M_1(G)$.

Let G^* be a unicyclic graph with the maximal first Zagreb index in $\mathbb{U}_r$ and let π be its degree sequence. Set $r_i = r_i(G^*)$ for each $1 \leq i \leq \Delta(G^*)$.

Claim 1. $\Delta(G^*) \geq 3$.

Proof. Suppose to the contrary that $\Delta(G^*) \leq 2$. Then $G^* = C_r$. Note that $F_{r+2}^k \in \mathbb{U}_r$ ($3 \leq k \leq r+1$), but

$$M_1(F_{r+2}^k) - M_1(C_r) = 4r + 10 - 4r = 10 > 0,$$

contradicting the maximality of G^* . □

Claim 2. $r_1 \geq r_2$.

Proof. Suppose to the contrary that $r_1 < r_2$. Let G_1 be the unicyclic graph obtained from G^* by adding a new vertex w and joining w to one maximum degree vertex x of G^* . Since $r_1 < r_2$, we have $r_1 + 1 \leq r_2$, so $\text{rep}(G_1) = r_2 = r$; hence $G_1 \in \mathbb{U}_r$. However,

$$M_1(G_1) - M_1(G^*) = (d_{G^*}(x) + 1)^2 - d_{G^*}^2(x) + 1 = 2d_{G^*}(x) + 2 > 0,$$

contradicting the maximality of G^* . □

Claim 3. $r_2 \geq r_1$.

Proof. Suppose to the contrary that $r_2 < r_1$. Let x be a pendent vertex of G^* and y be the unique neighbor of x . Let G_2 be the unicyclic graph obtained from G^* by inserting a new vertex w on the edge xy . Since $r_2 < r_1$, we have $r_2 + 1 \leq r_1$, so $\text{rep}(G_2) = r_1 = r$; hence $G_2 \in \mathbb{U}_r$. However,

$$M_1(G_2) - M_1(G^*) = d_{G_2}^2(w) = 4,$$

contradicting the maximality of G^* . □

By Claim 1, we have $G^* \neq C_r$. By Claims 2 and 3 and Lemma 2.1, we have

$$(3.1) \quad r_1 = r_2 = \text{rep}(G^*) = r.$$

Assume that G^* has s vertices of degree at least three. By Claim 1 and (3.1), $s \geq 1$ and G^* has exactly $s + 2r$ vertices. Further, we may assume that $\pi = (d_1, d_2, \dots, d_{s+2r})$ and

$$d_1 \geq d_2 \geq \dots \geq d_s \geq 3 > d_{s+1} = \dots = d_{s+r} = 2 > d_{s+r+1} = \dots = d_{s+2r} = 1.$$

Since G^* is unicyclic, $|E(G^*)| = |V(G^*)| = s + 2r$. By the handshaking lemma, the sum of all degrees in G^* equals

$$\sum_{v \in V(G^*)} d_{G^*}(v) = 2|E(G^*)| = 2(s + 2r).$$

On the other hand, summing the degrees according to the three degree classes gives

$$\sum_{v \in V(G^*)} d_{G^*}(v) = \sum_{i=1}^s d_i + 2r + r,$$

where $\sum_{i=1}^s d_i$ is the contribution of the vertices of degree at least 3, $2r$ is the contribution of the r vertices of degree 2, and r is the contribution of the r vertices of degree 1. Combining these two expressions yields

$$\sum_{i=1}^s d_i + 2r + r = 2(s + 2r).$$

Hence

$$\sum_{i=1}^s d_i = 2s + r,$$

or equivalently,

$$\sum_{i=1}^s (d_i - 2) = r.$$

Therefore $(d_1 - 2, d_2 - 2, \dots, d_s - 2)$ is a partition of r . Consequently,

$$M_1(G^*) = \sum_{i=1}^s d_i^2 + 4r + r = \sum_{i=1}^s d_i^2 + 5r = \sum_{i=1}^s ((d_i - 2) + 2)^2 + 5r \leq f(r) + 5r,$$

by the definition of the function $f(r)$.

In conclusion, $M_1(G) \leq f(r) + 5r$ for any unicyclic graph G with girth at least 3 and $G \in \mathbb{U}_r$. Since $r \geq 5$, by Lemma 2.2, $f(r) = (r + 2)^2$. Thus, if G^* is a unicyclic graph satisfying the upper bound, then G^* has degree sequence

$$(r + 2, \underbrace{2, \dots, 2}_r, \underbrace{1, \dots, 1}_r).$$

This completes the proof of Theorem 1.2.

4. Conclusions

In this paper, we bound the first Zagreb index of unicyclic graphs from both below and above by expressions depending uniquely on their repetition number and determine the degree sequences for these graphs with the largest and smallest first Zagreb indices, respectively.

Remark 1. In Theorem 1.1, if T^* is a tree satisfying the upper bound, then $r_1(T^*) = r_2(T^*) = \text{rep}(T^*)$. In fact, by Lemma 2.2, if $r \geq 7$ and T^* is a tree satisfying the upper bound, then T^* has degree sequence

$$(r, \underbrace{2, \dots, 2}_r, \underbrace{1, \dots, 1}_r).$$

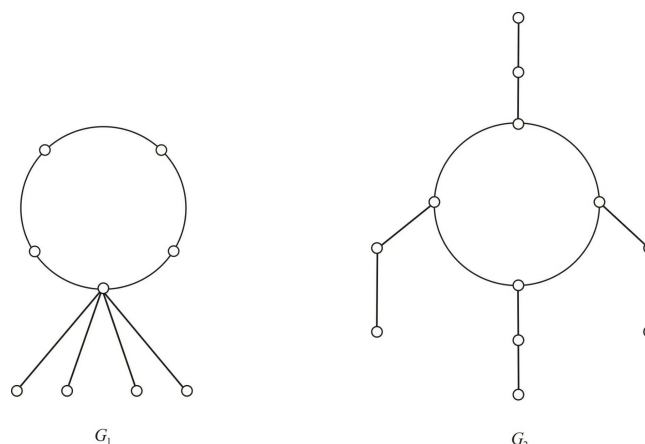


FIGURE 2. Two unicyclic graphs G_1 and G_2 in $\mathbb{U}_4$ with maximum value of $M_1 = 56$.

Remark 2. We remark that in Theorem 1.2, for $r = 3, 4$, we also have $4r \leq M_1(G) \leq f(r) + 5r$. But for some specific integers $r \leq 4$, the extremal unicyclic graphs in $\mathbb{U}_r$ realizing the upper bound might have different numbers of vertices. In the case $r = 4$, the set of all partitions of 4 is

$$\mathcal{P}(4) = \{(4), (3, 1), (2, 2), (2, 1, 1), (1, 1, 1, 1)\}.$$

It is easily checked that $f(r) = f(4) = 36$ is attained by two partitions (4) and (1, 1, 1, 1). In the class $\mathbb{U}_4$, the maximum value of M_1 is $f(r) + 5r = f(4) + 20 = 56$. In Figure 2, two unicyclic graphs in $\mathbb{U}_4$ with maximum value of M_1 are depicted. The unicyclic graph G_1 has 9 vertices and the degree sequence (6, 2, 2, 2, 2, 1, 1, 1, 1), while the unicyclic graph G_2 possesses 12 vertices and the degree sequence (3, 3, 3, 3, 2, 2, 2, 2, 1, 1, 1, 1).

Acknowledgments

The authors would like to thank anonymous referees for careful reading and valuable suggestions to improve the manuscript. This work is supported by the National Natural Science Foundation of China [Grant No. 12301455] and Natural Science Foundation of Shandong Province [Grant Nos. ZR2023QA080, ZR2024MA073].

REFERENCES

- [1] A. Ali, I. Gutman, E. Milovanović and I. Milovanović, Sum of powers of the degrees of graphs: extremal results and bounds, *MATCH Commun. Math. Comput. Chem.*, **80** no. 1 (2018) 5–84.
- [2] B. Borovićanin, On the extremal Zagreb indices of trees with given number of segments or given number of branching vertices, *MATCH Commun. Math. Comput. Chem.*, **74** no. 1 (2015) 57–79.
- [3] Y. Caro and D. B. West, Repetition number of graphs, *Electron. J. Combin.*, **16** no. 1 (2009) Research Paper 7, 14 pp.

- [4] H. Deng, A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs, *MATCH Commun. Math. Comput. Chem.*, **57** no. 3 (2007) 597–616.
- [5] P. Das, K. C. Das, S. Mondal and A. Pal, First Zagreb spectral radius of unicyclic graphs and trees, *J. Comb. Optim.*, **48** no. 1 Paper No. 5, 24 pp.
- [6] S. Filipovski, New bounds for the first Zagreb index, *MATCH Commun. Math. Comput. Chem.*, **85** no. 2 (2021) 303–312.
- [7] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. Total π -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.
- [8] I. Gutman, B. Rušćić, N. Trinajstić and C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys.*, **62** (1975) 3399–3405.
- [9] I. Gutman and M. Goubko, Trees with fixed number of pendent vertices with minimal first Zagreb index, *Bull. Int. Math. Virt. Inst.*, **3** no. 2 (2013) 161–164.
- [10] I. Gutman and K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.*, No. 50 (2004) 83–92.
- [11] T. Vetrík and S. Balachandran, General multiplicative Zagreb indices of trees and unicyclic graphs with given matching number, *J. Comb. Optim.*, **40** no. 4 (2020) 953–973.
- [12] H. Lin, On segments, vertices of degree two and the first Zagreb index of trees, *MATCH Commun. Math. Comput. Chem.*, **72** no. 3 (2014) 825–834.
- [13] H. Lin and J. Qian, Bounding the first Zagreb index of a tree in terms of its repetition number, *MATCH Commun. Math. Comput. Chem.*, **89** no. 3 (2023) 723–731.
- [14] S. Zhang and H. Zhang, Unicyclic graphs with the first three smallest and largest first general Zagreb index, *MATCH Commun. Math. Comput. Chem.*, **55** no. 2 (2006) 427–438.

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