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A Degree-Based Spectral Radius Conjecture Refuted: The Second Zagreb Matrix of Unicyclic Graphs

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Abstract

A conjecture in [MATCH Commun. Math. Comput. Chem. **89** (2023) 513–530] states that for any unicyclic graph G of order $n \geq 3$, the spectral radius of any degree–based matrix (i.e., a matrix whose entries are functions of vertex degrees) lies between $\rho(C_n)$ and $\rho(S_3^+)$, where S_3^+ denotes the unicyclic graph obtained by attaching $n-3$ pendent vertices to a single vertex of a triangle. We disprove the upper bound for the second Zagreb matrix. Exhaustive computations for $n = 5$ to 11 show that the true maximizer is a triangle: for $n = 6$ it has one leaf on each vertex $(1, 1, 1)$; for all other $n \geq 5$ it has leaf counts $(\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil, 0)$ (i.e., one cycle vertex receives no pendent leaf). We conjecture that these graphs uniquely maximize the second Zagreb spectral radius for every $n \geq 5$.

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1 Introduction

The second Zagreb matrix $Z_e(G)$ of a graph G is defined by $(Z_e)_{ij} = d_i d_j$ if $v_i \sim v_j$ and 0 otherwise; its spectral radius is denoted $\rho(G)$ [4]. For unicyclic graphs, a conjecture stated in [6] asserts that for any degree–based matrix, $\rho(C_n) \leq \rho(G) \leq \rho(S_3^+)$ (where S_3^+ is a triangle with $n-3$ pendent leaves attached to one vertex). We show that the upper bound fails for the second Zagreb matrix.

2 Lower bound

For an irreducible non–negative matrix, the spectral radius lies between the minimum and maximum row sums. For $Z_e(G)$, the i-th row sum is $R_i = d_i \sum_{j\sim i} d_j$, and $\sum_i R_i = 2M_2(G)$. It is known that $M_2(G) \geq 4n$ for any unicyclic G, with equality iff $G \cong C_n$. Hence $\rho(G) \geq \frac{2}{n} M_2(G) \geq 8 = \rho(C_n)$, proving the lower bound.

3 Counterexamples to the original conjecture and the true maximizers

We computed the second Zagreb spectral radii of all connected unicyclic graphs of orders 5 through 11. For each graph, the unique cycle is a triangle. Let (a, b, c) denote the numbers of pendent leaves attached to the three vertices of the triangle (in any order). The results, summarized in Table 1, show that the upper bound $\rho(G) \leq \rho(S_3^+)$ fails for every $n \geq 5$. Moreover, the extremal graphs follow a clear pattern.

For $n = 5, 7, 8, 9, 10, 11$ the extremal graph is a triangle where one vertex receives no pendent leaf (i.e., $c = 0$ up to permutation), and the remaining $n-3$ leaves are distributed between the other two vertices as evenly as possible (so $|a - b| \leq 1$). For $n = 6$ the unique maximizer is the triangle with one leaf on each vertex, i.e., $(1, 1, 1)$.

Table 1. Second Zagreb spectral radii of S_3^+ and the true maximizers for $n = 5, \ldots, 11$.

n	(a, b, c)	$\rho(S_3^+)$	$\max \rho(G)$	$\rho(C_n)$
5	(1,1,0)	14.456	**14.562**	8.000
6	(1,1,1)	18.202	**18.487**	8.000
7	(2,2,0)	22.251	**22.967**	8.000
8	(2,3,0)	26.579	**27.797**	8.000
9	(3,3,0)	31.167	**33.267**	8.000
10	(3,4,0)	36.000	**39.036**	8.000
11	(4,4,0)	41.065	**45.495**	8.000

Let G_n^* denote this family:

$$G_n^* = \begin{cases} \text{triangle with leaf counts } (1,1,1), & n = 6, \\ \text{triangle with leaf counts } \left(\lfloor \frac{n-3}{2} \rfloor,\ \lceil \frac{n-3}{2} \rceil,\ 0\right), & n \neq 6,\ n \geq 5. \end{cases}$$

Based on these data, we propose the following corrected conjecture.

Conjecture 1. *For every unicyclic graph G of order $n \geq 5$,*

$$\rho(G) \ \leq \ \rho(G_n^*),$$

with equality if and only if $G \cong G_n^*$.

Heuristic justification: The triangle maximizes cycle–vertex degrees. For $n \geq 7$ it becomes optimal to leave one cycle vertex without pendent leaves, because attaching leaves to all three vertices forces the degrees to be lower on two of them, reducing the product $d_i d_j$ on the cycle edges. The remaining leaves are then split between the two other cycle vertices to balance the row sums of the second Zagreb matrix, in agreement with the Frobenius bound.

4 Conclusion

We disproved the upper bound $\rho(G) \leq \rho(S_3^+)$ for the second Zagreb matrix of unicyclic graphs. Computations for $n = 5$–11 show that the true maximizer is:

- for $n = 6$: triangle $(1, 1, 1)$;
- for $n \neq 6$, $n \geq 5$: triangle $(\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil, 0)$.

We conjecture that these graphs G_n^* are the unique extremal graphs for all $n \geq 5$.

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