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On a conjecture about the second Zagreb index

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Abstract

The cyclomatic number ν of a graph G is the minimum number of those edges of G whose removal makes G as acyclic. The second Zagreb index M_2 for a graph G is the sum of the products of degrees of adjacent vertices of G. For $\nu = \binom{k-1}{2} + t$ with $1 \le t \le k-1$ and $4 \le k \le n-2$, let G^* be the graph having maximum M_2 value in the class of all connected graphs with order n and cyclomatic number ν. Xu *et al.* [*MATCH Commun. Math. Comput. Chem.* **72** (2014) 641–654] posed a conjecture concerning the exact structure of the graph G^*. In this note, a partial progress is made on this conjecture by proving that G^* has a specific type of subgraph with the size $\binom{k-1}{2} + t$ and minimum degree at least one.

Keywords: second Zagreb index; cyclomatic number; extremal problem.

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1. Introduction

Every graph considered in this note is simple and finite. The vertex set and edge set of a graph G will be denoted by $V(G)$ and $E(G)$, respectively. Edge connecting the vertices $u, v \in V(G)$ and the degree of a vertex u will be denoted by uv and $d_u(G)$ (or d_u, when there is no confusion), respectively. A pendant vertex of a graph is a vertex with degree 1. By an n-vertex graph, we mean a graph of order n. The cyclomatic number of a graph G, denoted by $\nu(G)$ (or ν, when there is no confusion), is the minimum number of those edges of G whose removal makes G as acyclic. Denote by $\mathbb{G}_{n,\nu}$ the class of all n-vertex connected graphs with cyclomatic number ν. By saying that two graphs G and H are disjoint, we mean that the graphs G and H are vertex-disjoint as well as edge-disjoint. The union and join of two graphs G_1, G_2 will be denoted by $G_1 \cup G_2$ and $G_1 + G_2$, respectively. Throughout this note, union and join will be taken over disjoint graphs. Denote by rK_1 the union of r isolated vertices. The set of all vertices adjacent to a vertex $u \in V(G)$ will be denoted by $N_G(u)$. Undefined terminology and notation from graph theory can be found in some standard books, like [3, 9].

The second Zagreb index M_2 (appeared in [7] within the study of molecular branching) for a graph G is defined as

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

Although the mathematical theory of the second Zagreb index is well-documented (for example, see the recent survey paper [4] and the related references listed therein), some interesting extremal graph-theoretical problems regarding this index are still open. One of these open problems is the problem of finding graph(s) with the maximal second Zagreb index in the graph class $\mathbb{G}_{n,\nu}$. Indeed, a partial progress on the solution of this open problem has already been made: Deng [6] solved this problem for $\nu \le 2$; Xu *et al.* [10] gave the solution of this problem for the cases $\nu \le 3$ and $\nu = \binom{k-1}{2}$, where $4 \le k \le n-2$, and also they posed the following conjecture regarding this problem.

Conjecture 1.1. [10] *Let $\nu = \binom{k-1}{2} + t$ where $1 \le t \le k-1$ and $4 \le k \le n-2$. The graph $K_k^{n-k}(t)$ has the maximum M_2 value among all the graphs of $\mathbb{G}_{n,\nu}$, where $K_k^{n-k}(t)$ is the graph obtained from $[K_{k-1} \cup (n-k)K_1] + K_1$ by adding t new edges between a fixed pendant vertex and t other vertices of degree $k-1$.*

In [1, 8], it was proved that Conjecture 1.1 holds for $\nu = 4$. Recently, in [2], this conjecture was proved for the case $\nu = 5$. In this note, a partial progress is made on Conjecture 1.1 by proving that the graph having maximum M_2 value in the class $\mathbb{G}_{n,\nu}$, has a specific type of subgraph with the size $\binom{k-1}{2} + t$ and minimum degree at least one, where $\nu = \binom{k-1}{2} + t$ with $1 \le t \le k-1$ and $4 \le k \le n-2$.

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2. Main results

In order to state and prove the main results, we need two already known lemmas. The first of these two lemmas is the following one, which is due to Xu *et al.* [10].

Lemma 2.1. [10] *Let $\nu = \binom{k-1}{2} + t$ where $1 \le t \le k-1$ and $4 \le k \le n-2$. If G is the graph with the maximum M_2 value in $\mathbb{G}_{n,\nu}$ then the maximum degree of G is $n-1$.*

For stating the next lemma, we need some definitions and notations. Let

$$M^*(G) = \sum_{uv \in E(G)} (d_u + 1)(d_v + 1).$$

For the simplicity, we write $d_i = d_{v_i}$ for $v_i \in V(G)$. In what follows, we recall the definition of a graph class, given in [5]. Let $\widetilde{G} = G(d_1, d_2, \dots, d_N)$ be a graph with the vertex set

$$\bigcup_{j=0}^{N} I_j,$$

as a disjoint union, where $I_0 = \{v_1, v_2, \dots, v_N\}$, $|I_j| = d_j - d_{j+1}$ for $j = 1, 2, \dots, N-1$, $|I_N| = d_N - (N-1)$ and $d_1 \ge d_2 \ge \cdots \ge d_N \ge N-1$. Also, for $j = 1, 2, \dots, N$, we take

$$N_{\widetilde{G}}(v_j) = (I_0 \setminus \{v_j\}) \cup \left(\bigcup_{k=j}^{N} I_k \right)$$

and assume that all the vertices of the set

$$\bigcup_{j=1}^{N} I_j$$

are pairwise non-adjacent. The graph $\widetilde{G}$ is shown in Figure 1. It is clear that the size of the graph $\widetilde{G}$ is

$$\sum_{i=1}^{N} d_i - \binom{N}{2}.$$

Denote by $\mathfrak{F}$ the class of all graphs of the form $\widetilde{G}$.

Lemma 2.2. [5] *Let k' and t be positive integers with $1 \le t \le k'$. If G is a graph of minimal degree at least one and has maximum M^* value among all the graphs of size $\binom{k'}{2} + t$, then $G \in \mathfrak{F}$.*

Now, we are ready to state and prove the first main result of the present note.

Proposition 2.1. *Let $\nu = \binom{k-1}{2} + t$ where $1 \le t \le k-1$ and $4 \le k \le n-2$. If G is a graph with the maximal M_2 value among all the graphs of $\mathbb{G}_{n,\nu}$ then $G \cong (H \cup sK_1) + K_1$ and*

$$M_2(G) = (n-1)(n + 2t + k^2 - 3k + 1) + M^*(H). \tag{1}$$

where $H \in \mathfrak{F}$ and s is some non-negative integer.

Proof. By Lemma 2.1, the graph G must have a vertex of degree $n-1$. If $v \in V(G)$ is a vertex of degree $n-1$ then order and size of the graph $G - v$ are

$$n-1 \quad \text{and} \quad \binom{k-1}{2} + t,$$

respectively, where $1 \le t \le k-1$, $4 \le k \le n-2$. By using the definition of the second Zagreb index, we have

$$\begin{aligned} M_2(G) &= d_v(G) \sum_{x \in V(G-v)} d_x(G) + \sum_{uw \in V(G-v)} d_u(G) d_w(G) \\ &= d_v(G) \sum_{x \in V(G-v)} (d_x(G-v) + 1) + \sum_{uw \in V(G-v)} (d_u(G-v) + 1)(d_w(G-v) + 1) \\ &= (n-1)(n + 2t + k^2 - 3k + 1) + M^*(G-v). \end{aligned} \tag{2}$$

It is evident that if H is the graph obtained from $G - v$ by removing all isolated vertices (if H does not contain any isolated vertex, we take $H \cong G - v$), then

$$M^*(G-v) = M^*(H). \tag{3}$$

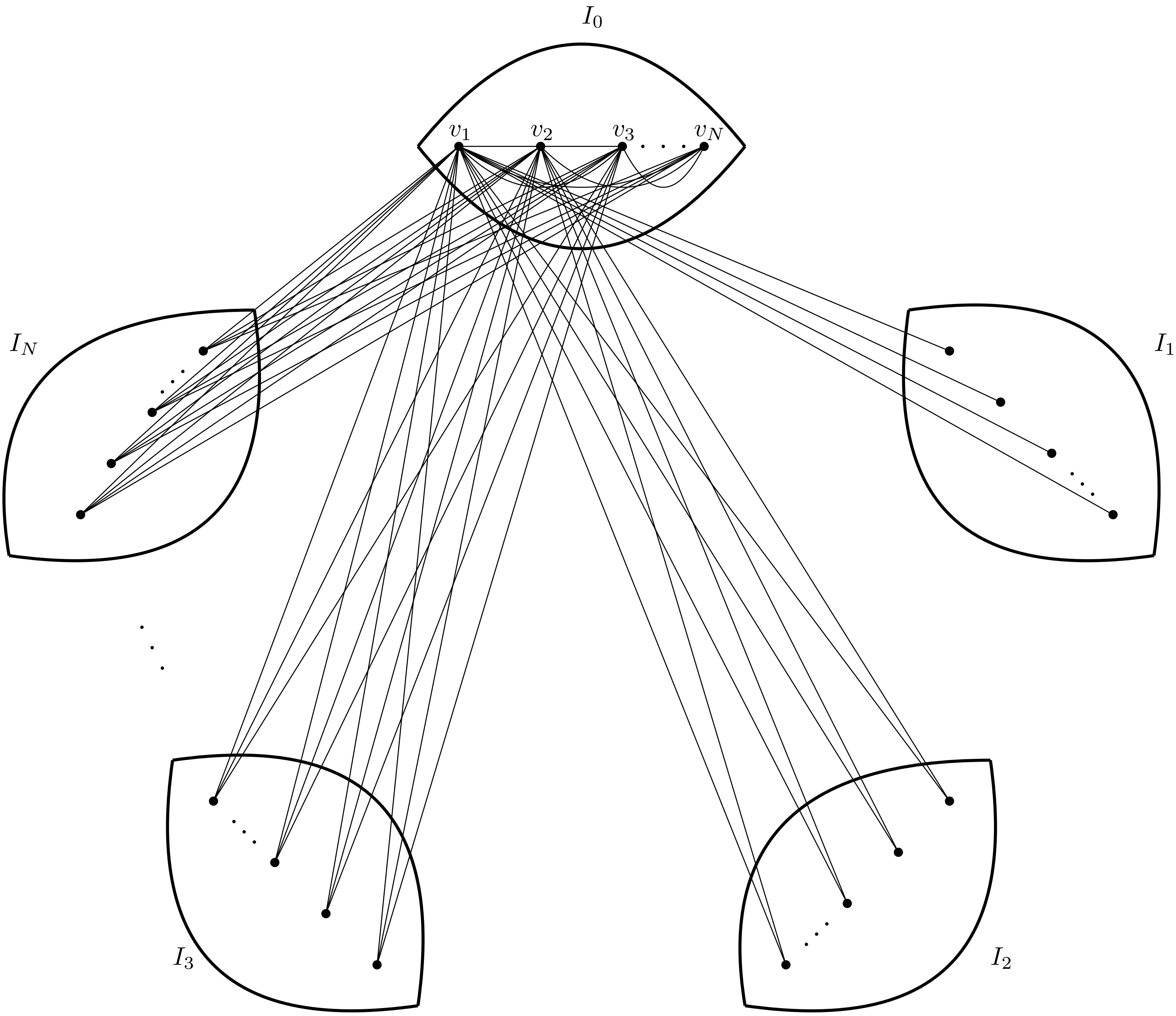

Figure 1: The graph $\widetilde{G}$.

Bearing in mind the definition of G, from Equations (2) and (3), we conclude that H must have the maximal M^* value among all the graphs of size $\binom{k'}{2}+t$, where $1 \le t \le k'$ and $k' = k-1$. But then, Lemma 2.2 ensures that H belongs to the class $\mathfrak{F}$.

□

Because of Equation (1), in order to determine the graph with the maximal M_2 value in $\mathbb{G}_{n,\nu}$, it is enough to find the graph having maximum M^* value in the graph class $\mathfrak{F}$. Thus, Conjecture 1.1 will be true if the following conjecture holds.

Conjecture 2.1. *If a graph G has the maximum M^* value among all the graphs of $\mathfrak{F}$ with the size $\binom{k-1}{2}+t$ where $1 \le t \le k-1$ and $4 \le k \le n-2$, then G is isomorphic to the graph consisting of the $(k-1)$-vertex complete graph K_{k-1} together with an additional vertex joined to t vertices of K_{k-1}.*

The first step towards Conjecture 2.1 is the next proposition, which gives M^* value of an arbitrary graph of $\mathfrak{F}$.

Proposition 2.2. *If $G \in \mathfrak{F}$ then*

$$M^*(G) = \sum_{i=1}^{N} i\,(d_i+1)^2 + \left(\sum_{i=1}^{N} d_i\right)^2 - N(N-1)\sum_{i=1}^{N} d_i - N^3.$$

Proof. Suppose that the set A contains all those edges of G whose one end vertex belongs to I_0 and the other one belongs to I_j for some $1 \le j \le N$, and let $B = E(G) \setminus A$. We take

$$\Lambda_1 = \sum_{uv \in A} (d_u + 1)(d_v + 1) \text{ and } \Lambda_2 = \sum_{uv \in B} (d_u + 1)(d_v + 1),$$

then $M^*(G) = \Lambda_1 + \Lambda_2$. For the edges of A, we have

$$\begin{aligned}
|I_1| &= d_1 - d_2,\\
|I_2| &= d_2 - d_3,\\
|I_3| &= d_3 - d_4,\\
&\vdots\\
|I_{N-1}| &= d_{N-1} - d_N,\\
|I_N| &= d_N - (N-1).
\end{aligned}$$

Hence,

$$\begin{aligned}
\Lambda_1 &= (d_1 - d_2)(2d_1 + 2) + (d_2 - d_3)\left(3\sum_{i=1}^{2} d_i + 6\right) + (d_3 - d_4)\left(4\sum_{i=1}^{3} d_i + 12\right)\\
&\quad + \cdots + (d_{N-1} - d_N)\left(N\sum_{i=1}^{N-1} d_i + N(N-1)\right)\\
&\quad + (d_N - (N-1))\left((N+1)\sum_{i=1}^{N} d_i + N(N+1)\right)\\
&= \Bigg[2d_1(d_1 - d_2) + (d_2 - d_3)\left(3\sum_{i=1}^{2} d_i\right) + (d_3 - d_4)\left(4\sum_{i=1}^{3} d_i\right)\\
&\quad + \cdots + (d_{N-1} - d_N)\left(N\sum_{i=1}^{N-1} d_i\right) + (d_N - (N-1))\left((N+1)\sum_{i=1}^{N} d_i\right)\Bigg]\\
&\quad + \Big[2(d_1 - d_2) + 6(d_2 - d_3) + 12(d_3 - d_4) + \cdots + N(N-1)(d_{N-1} - d_N)\\
&\quad + N(N+1)(d_N - (N-1))\Big]\\
&= \Bigg[\left(2d_1^2 + 3d_2\sum_{i=1}^{2} d_i + 4d_3\sum_{i=1}^{3} d_i + \cdots + Nd_{N-1}\sum_{i=1}^{N-1} d_i + (N+1)d_N\sum_{i=1}^{N} d_i\right)\\
&\quad - \left(\left(2d_1d_2 + 3d_3\sum_{i=1}^{2} d_i + 4d_4\sum_{i=1}^{3} d_i + \cdots + Nd_N\sum_{i=1}^{N-1} d_i\right) + (N^2 - 1)\sum_{i=1}^{N} d_i\right)\Bigg]\\
&\quad + \Big[2d_1 + 4d_2 + 6d_3 + \cdots + 2Nd_N - N(N^2 - 1)\Big]\\
&= \Bigg[\left(2d_1^2 + 3d_2^2 + 4d_3^2 + \cdots + (N+1)d_N^2\right)\\
&\quad + \left(\left(d_1d_2 + d_3\sum_{i=1}^{2} d_i + d_4\sum_{i=1}^{3} d_i + \cdots + d_N\sum_{i=1}^{N-1} d_i\right) - (N^2 - 1)\sum_{i=1}^{N} d_i\right)\Bigg]\\
&\quad + \left[2\sum_{i=1}^{N} i d_i - N(N^2 - 1)\right]\\
&= \sum_{i=1}^{N}(i+1)d_i^2 - (N^2 - 1)\sum_{i=1}^{N} d_i + 2\sum_{i=1}^{N} i d_i - N(N^2 - 1)\\
&\quad + \left(d_1d_2 + d_3\sum_{i=1}^{2} d_i + d_4\sum_{i=1}^{3} d_i + \cdots + d_N\sum_{i=1}^{N-1} d_i\right)
\end{aligned}$$

Now, we calculate Λ_2 as follows

$$\Lambda_2 = (d_1 + 1)\left(\sum_{i=2}^{N} d_i + (N-1)\right) + (d_2 + 1)\left(\sum_{i=3}^{N} d_i + (N-2)\right)$$

$$
\begin{aligned}
&+(d_3+1)\left(\sum_{i=4}^{N} d_i+(N-3)\right)+\cdots+(d_{N-1}+1)\left(\sum_{i=N}^{N} d_i+1\right)\\
=\;&[(N-1)(d_1+1)+(N-2)(d_2+1)+(N-3)(d_3+1)+\cdots+(d_{N-1}+1)]\\
&+\left(d_1\sum_{i=2}^{N} d_i+d_2\sum_{i=3}^{N} d_i+d_3\sum_{i=4}^{N} d_i+\cdots+d_{N-1}\sum_{i=N}^{N} d_i\right)\\
&+\left(\sum_{i=2}^{N} d_i+\sum_{i=3}^{N} d_i+\sum_{i=4}^{N} d_i+\cdots+\sum_{i=N}^{N} d_i\right)\\
=\;&\left[((N-1)d_1+(N-2)d_2+(N-3)d_3+\cdots+2d_{N-2}+d_{N-1})+\frac{N(N-1)}{2}\right]\\
&+\left(d_1\sum_{i=2}^{N} d_i+d_2\sum_{i=3}^{N} d_i+d_3\sum_{i=4}^{N} d_i+\cdots+d_{N-1}\sum_{i=N}^{N} d_i\right)\\
&+\left(\sum_{i=2}^{N} d_i+\sum_{i=3}^{N} d_i+\sum_{i=4}^{N} d_i+\cdots+\sum_{i=N}^{N} d_i\right)\\
=\;&\left(d_1\sum_{i=2}^{N} d_i+d_2\sum_{i=3}^{N} d_i+d_3\sum_{i=4}^{N} d_i+\cdots+d_{N-1}\sum_{i=N}^{N} d_i\right)\\
&+(N-1)\sum_{i=1}^{N} d_i+\frac{N(N-1)}{2}
\end{aligned}
$$

Finally, we have

$$
\begin{aligned}
M^*(G) &= \Lambda_1+\Lambda_2\\
&= \sum_{i=1}^{N} i d_i^2-N(N-1)\sum_{i=1}^{N} d_i+2\sum_{i=1}^{N} i d_i-\frac{N(N-1)(2N+1)}{2}\\
&\quad+\Bigg[\sum_{i=1}^{N} d_i^2+\left(d_1d_2+d_3\sum_{i=1}^{2} d_i+d_4\sum_{i=1}^{3} d_i+\cdots+d_N\sum_{i=1}^{N-1} d_i\right)\\
&\quad+\left(d_1\sum_{i=2}^{N} d_i+d_2\sum_{i=3}^{N} d_i+d_3\sum_{i=4}^{N} d_i+\cdots+d_{N-1}\sum_{i=N}^{N} d_i\right)\Bigg]\\
&= \sum_{i=1}^{N} i d_i^2-N(N-1)\sum_{i=1}^{N} d_i+2\sum_{i=1}^{N} i d_i-\frac{N(N-1)(2N+1)}{2}\\
&\quad+\Bigg[d_1\left(d_1+\sum_{i=2}^{N} d_i\right)+d_2\left(d_1+d_2+\sum_{i=3}^{N} d_i\right)+d_3\left(\sum_{i=1}^{2} d_i+d_3+\sum_{i=4}^{N} d_i\right)\\
&\quad+\cdots+d_N\left(d_N+\sum_{i=1}^{N-1} d_i\right)\Bigg]\\
&= \sum_{i=1}^{N} i d_i^2-N(N-1)\sum_{i=1}^{N} d_i+2\sum_{i=1}^{N} i d_i-\frac{N(N-1)(2N+1)}{2}+\left(\sum_{i=1}^{N} d_i\right)^2,
\end{aligned}
$$

which gives the required result. □

From Propositions 2.1 and 2.2, the next result follows.

Proposition 2.3. *Let $\nu=\binom{k-1}{2}+t$ where $1\le t\le k-1$ and $4\le k\le n-2$. If G is a graph with the maximal M_2 value among all the graphs of $\mathbb{G}_{n,\nu}$ then $G\cong(\widetilde{G}\cup sK_1)+K_1$ and*

$$M_2(G)=\sum_{i=1}^{N} i\,(d_i+1)^2+\left(\sum_{i=1}^{N} d_i\right)^2-N(N-1)\sum_{i=1}^{N} d_i-N^3+(n-1)(n+2t+k^2-3k+1).$$

where $\widetilde{G}=G(d_1,d_2,\ldots,d_N)\in\mathfrak{F}$ and s is some non-negative integer.

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