

Research Article

Exponential second Zagreb index of connected graphs

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(Received: 18 August 2025. Received in revised form: 2 October 2025. Accepted: 7 October 2025. Published online: 28 October 2025.)

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Abstract

For a graph $G = (V, E)$, the exponential second Zagreb index is defined as $e^{M_2}(G) = \sum_{uv \in E(G)} e^{d_u d_v}$, where d_v denotes the degree of a vertex $v \in V(G)$. This paper addresses the problems of characterizing connected graphs of fixed order having the (i) maximum and minimum e^{M_2} with a given number of cut edges, (ii) maximum e^{M_2} with a given number of pendent vertices, (iii) minimum e^{M_2} with a given girth, and (iv) minimum e^{M_2} with a given maximum degree.

Keywords: exponential second Zagreb index; cut edge; pendent vertex.

2020 Mathematics Subject Classification: 05C07, 05C09.

1. Introduction

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For each vertex $v \in V(G)$, let d_v denote its degree, which is the number of edges incident to it, and let $N_G(v) = N(v)$ represent the set of vertices adjacent to v . The distance between two vertices is defined as the length of the shortest path connecting them, measured by the number of edges in that path. The diameter of a graph is the maximum distance between any pair of vertices in the graph.

The exponential version of the second Zagreb index, also known as the exponential second Zagreb index, was introduced by Rada [11] and is defined as

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

In [4], Cruz and Rada posed an open problem to determine the extremal trees that maximize the exponential second Zagreb index e^{M_2} among all trees of order n . This problem was independently resolved in several works [3, 5, 16]. In 2022, Eliasi [6] determined the extremal graphs that maximize the exponential second Zagreb index e^{M_2} among all unicyclic and bicyclic graphs of order n . He further proposed a conjecture regarding the characterization of extremal graphs that attain the maximum value of the exponential second Zagreb index among all graphs with n vertices and m edges, where $n \leq m \leq 2n - 3$. Xu et al. [15] confirmed the conjecture for all graphs whose diameter is different from three, and a complete solution was later provided in [2]. Moreover, the extremal graphs corresponding to other ranges of m were also characterized in [2]. Some recent studies on e^{M_2} can be found [1, 4, 11, 13, 14].

The problem of identifying extremal graphs—those that attain the maximum or minimum values of various topological indices—within classes defined by a fixed number of vertices and either a given number of cut edges or a specified number of pendent vertices has been extensively studied. For example, such investigations have been carried out with respect to the first and second Zagreb indices, the reduced second Zagreb index, and the Sombor index; see [7–10, 12], respectively.

It is worth noting that the extremal graphs maximizing the first and second Zagreb indices, as well as the Sombor index, coincide, while a slightly different graph arises in the case of the reduced second Zagreb index. In contrast, the graphs minimizing these indices are identical across all cases. However, for the exponential second Zagreb index, the structure of the extremal graph attaining the maximum value varies depending on whether the constraint is on the number of cut edges or the number of pendent vertices.

In this paper, we study the problems of characterizing connected graphs of fixed order having the (i) maximum and minimum e^{M_2} with a given number of cut edges, (ii) maximum e^{M_2} with a given number of pendent vertices, (iii) minimum e^{M_2} with a given girth, and (iv) minimum e^{M_2} with a given maximum degree.

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2. Graphs with the maximum exponential second Zagreb index

In this section, we consider classes of connected n -vertex graphs with given number of pendent vertices or cut edges. Denote $\mathcal{G}_n^p$ and $\mathcal{G}_n^{(k)}$ the class of connected n -vertex graphs with p pendent vertices and the class of connected n -vertex graphs with k cut edges, respectively. Let $p_1, p_2, \dots, p_s$ be non-negative integers and $G(p_1, p_2, \dots, p_s)$ be the obtained graph from a complete graph K_s with $V(K_s) = \{v_1, v_2, \dots, v_s\}$ by attaching p_i pendent vertices to v_i of K_s for $1 \leq i \leq s$. If $s = 1$ then $G(p_1) \cong S_{p_1+1}$. Hence if $n - p = 1$ then $\mathcal{G}_n^p = \{S_{p+1}\}$. Therefore, we assume that $n - p \geq 2$. For given positive integers n and p such that $1 \leq p \leq n - 2$, we set $q = n - p - 1$ and consider a function

$$g(t) = e^{(q+t)(q+p-t)} + (q-1) \left[e^{q(q+t)} + e^{q(q+p-t)} \right] + te^{q+t} + (p-t)e^{q+p-t},$$

on $0 \leq t \leq \lfloor p/2 \rfloor$. If $g(0) = g(\lfloor p/2 \rfloor)$ then the number e is a root of a polynomial

$$P(t) = t^{(q+\lfloor p/2 \rfloor)(q+\lceil p/2 \rceil)} + (q-1) \left(t^{q(q+\lfloor p/2 \rfloor)} + t^{q(q+\lceil p/2 \rceil)} \right) + \lfloor p/2 \rfloor t^{q+\lfloor p/2 \rfloor} + \lceil p/2 \rceil t^{q+\lceil p/2 \rceil} - qt^{q(q+p)} - (q-1)t^{q^2} - pt^{q+p},$$

and it contradicts that e is a transcendental number. Therefore, we have $g(0) \neq g(\lfloor p/2 \rfloor)$ for any integers p and q .

Theorem 2.1. *Let $e^{M_2}(G)$ be maximum in $\mathcal{G}_n^p$. Then*

$$e^{M_2}(G) = \max \{g(0), g(\lfloor p/2 \rfloor)\} + \binom{q}{2} e^{(n-p-1)^2}.$$

Moreover, the following hold:

- (i) if $g(0) < g(\lfloor p/2 \rfloor)$ then $G \cong G(\lceil p/2 \rceil, \lfloor p/2 \rfloor, 0, \dots, 0)$, where 0 occurs $n - p - 2$ times;
- (ii) if $g(0) > g(\lfloor p/2 \rfloor)$ then $G \cong G(p, 0, 0, \dots, 0)$, where 0 occurs $n - p - 1$ times.

Proof. Adding an edge in a graph, the exponential second Zagreb index of the graph is increasing. Therefore, one can easily see that there exist non-negative integers $p_1, p_2, \dots, p_{n-p}$ such that $p_1 + p_2 + \dots + p_{n-p} = p$ and $G \cong G(p_1, p_2, \dots, p_{n-p})$. Denote $d_i = p_i + n - p - 1$ for all $i = 1, 2, \dots, n - p$. Then we have

$$e^{M_2}(G) = e^{M_2}(G(p_1, p_2, \dots, p_{n-p})) = \sum_{i < j} e^{d_i d_j} + \sum_{i=1}^{n-k} p_i e^{d_i}.$$

Without loss of generality, we can assume that $p_1 \geq p_2 \geq p_3 \geq \dots \geq p_{n-p}$. If $p_3 > 0$ then

$$G' = G(p_1 + 1, p_2, p_3 - 1, p_4, \dots, p_{n-p}) \in \mathcal{G}_n^p$$

and

$$\begin{aligned} e^{M_2}(G') &= \sum_{j=4}^{n-p} \left[e^{(d_1+1)d_j} + e^{(d_3-1)d_j} + e^{d_2 d_j} \right] + e^{(d_1+1)d_2} + e^{(d_3-1)d_2} + e^{(d_1+1)(d_3-1)} \\ &\quad + \sum_{4 \leq i < j} e^{d_i d_j} + (p_1 + 1)e^{d_1+1} + p_2 e^{d_2} + (p_3 - 1)e^{d_3-1} + \sum_{i=4}^{n-k} p_i e^{d_i}. \end{aligned}$$

Hence, we obtain

$$\begin{aligned} e^{M_2}(G') - e^{M_2}(G) &= \sum_{j=4}^{n-p} \left[e^{(d_1+1)d_j} + e^{(d_3-1)d_j} - e^{d_1 d_j} - e^{d_3 d_j} \right] + e^{(d_1+1)d_2} + e^{(d_3-1)d_2} + e^{(d_1+1)(d_3-1)} - e^{d_1 d_2} - e^{d_3 d_2} - e^{d_1 d_3} \\ &\quad + (p_1 + 1)e^{d_1+1} + (p_3 - 1)e^{d_3-1} - p_1 e^{d_1} - p_3 e^{d_3}. \end{aligned} \quad (1)$$

Now we consider a function $f(x) = e^{(x+1)d_j} - e^{x d_j}$. Then $f'(x) = d_j f(x) > 0$ and it follows that $f(x)$ is increasing for $x \geq 0$. Therefore $e^{(d_1+1)d_j} + e^{(d_3-1)d_j} - e^{d_1 d_j} - e^{d_3 d_j} = f(d_1) - f(d_3 - 1) > 0$ since $d_1 > d_3 - 1$. From Equation (1), we have

$$\begin{aligned} e^{M_2}(G') - e^{M_2}(G) &> e^{(d_1+1)d_2} + e^{(d_3-1)d_2} + e^{(d_1+1)(d_3-1)} - e^{d_1 d_2} - e^{d_3 d_2} - e^{d_1 d_3} + (p_1 + 1)e^{d_1+1} + (p_3 - 1)e^{d_3-1} - p_1 e^{d_1} - p_3 e^{d_3} \\ &> e^{d_2} \cdot e^{d_1 d_2} - e^{d_1 d_2} - e^{d_3 d_2} - e^{d_1 d_3} + (p_1 + 1)e^{d_1} \cdot e - p_1 e^{d_1} - p_3 e^{d_3} > 0 \end{aligned}$$

since $e^{d_2} = e^{p_2+n-p-1} \geq e^2 > 3$ and $e(p_1 + 1) > p_1 + p_3$, where $n - p \geq 2$. This contradicts the fact that $e^{M_2}(G)$ attains its maximum value. Therefore, we have $p_3 = p_4 = \dots = p_{n-p} = 0$ and $p_1 + p_2 = p$. If $p \leq 3$ then we easily get the required result. Thus we assume that $p \geq 4$ and $\lfloor p/2 \rfloor - 1 \geq 1$.

Set $q = n - p - 1$ and recall that

$$g(t) = e^{(q+t)(q+p-t)} + (q-1) \left[e^{q(q+t)} + e^{q(q+p-t)} \right] + te^{q+t} + (p-t)e^{q+p-t},$$

where $0 \leq t \leq \lfloor p/2 \rfloor$. Hence we have

$$g''(t) = ((p-2t)^2 - 2)e^{(q+t)(q+p-t)} + (q-1)q^2 \left(e^{q(q+t)} + e^{q(q+p-t)} \right) + (t+2)e^{q+t} + (p-t+2)e^{q+p-t},$$

and it follows that $g(t)$ is strictly convex on the interval $0 \leq t \leq \lfloor p/2 \rfloor - 1$.

Let $g(x_0) \geq g(0)$ and $g(x_0) \geq g(\lfloor p/2 \rfloor - 1)$ for some x_0 such that $0 < x_0 < \lfloor p/2 \rfloor - 1$. Then by the definition of a strictly convex function, we have

$$g(x_0) = g((1-\alpha) \cdot 0 + \alpha(\lfloor p/2 \rfloor - 1)) < (1-\alpha)g(0) + \alpha g(\lfloor p/2 \rfloor - 1) \leq (1-\alpha)g(x_0) + \alpha g(x_0) = g(x_0),$$

where

$$\alpha = \frac{x_0}{\lfloor p/2 \rfloor - 1} < 1.$$

From this, we conclude that G is isomorphic to one of the following three graphs:

$$G(p, \underbrace{0, \dots, 0}_{n-p-1}), \quad G(\lceil p/2 \rceil + 1, \lfloor p/2 \rfloor - 1, \underbrace{0, \dots, 0}_{n-p-2}), \quad G(\lceil p/2 \rceil, \lfloor p/2 \rfloor, \underbrace{0, \dots, 0}_{n-p-2}).$$

It remains to show that

$$e^{M_2}(G(\lceil p/2 \rceil + 1, \lfloor p/2 \rfloor - 1, \underbrace{0, \dots, 0}_{n-p-2})) < e^{M_2}(G(\lceil p/2 \rceil, \lfloor p/2 \rfloor, \underbrace{0, \dots, 0}_{n-p-2})).$$

It is equivalent to $g(\lfloor p/2 \rfloor - 1) < g(\lfloor p/2 \rfloor)$. Set $a = \lfloor p/2 \rfloor$. Then

$$\begin{aligned} g(a) - g(a-1) &= e^{(q+a)(q+p-a)} - e^{(q+a-1)(q+p-a+1)} + (q-1) \left[e^{q(q+a)} - e^{q(q+a-1)} + e^{q(q+p-a)} - e^{q(q+p-a+1)} \right] \\ &\quad + ae^{q+a} - (a-1)e^{q+a-1} + (p-a)e^{q+p-a} - (p-a+1)e^{q+p-a+1} \\ &> e^{(q+a-1)(q+p-a+1)}(e^{p-2a+1} - 1) - (q-1)e^{q(q+p-a+1)} - (p-a+1)e^{q+p-a+1} \\ &\geq e^{(q+a-1)(q+p-a+1)}(e-1) - (q-1)e^{q(q+p-a+1)} - (p-a+1)e^{q+p-a+1} \\ &= e^{q+p-a+1} \left[e^{(q+a-2)(q+p-a+1)}(e-1) - (q-1)e^{(q-1)(q+p-a+1)} - (p-a+1) \right] \\ &> e^{(q+a-2)(q+p-a+1)}(e-1) - (q-1)e^{(q-1)(q+p-a+1)} - (p-a+1) \\ &> e^{q(q+p-a+1)} - (q-1)e^{(q-1)(q+p-a+1)} - (p-a+1) \\ &= e^{(q-1)(q+p-a+1)} \left[e^{q+p-a+1} - (q-1) \right] - p + a - 1 \\ &\geq e^{q+p-a+1} - (q-1) - p + a - 1 > 1 + (q+p-a+1) - (q-1) - p + a - 1 > 0 \end{aligned}$$

since $p - 2a \geq 0$, $e^{q+p-a+1} > 1$, $e^{(q-1)(q+p-a+1)} \geq 1$ and $e^{q+p-a+1} > 1 + (q+p-a+1)$. $\square$

Proposition 2.1. Let G be a graph of order n with m edges and k cut edges. If $e^{M_2}(G)$ is maximum in the class of graphs of order n with m edges and k cut edges. Then the number of non-pendent cut edges in G is at most one.

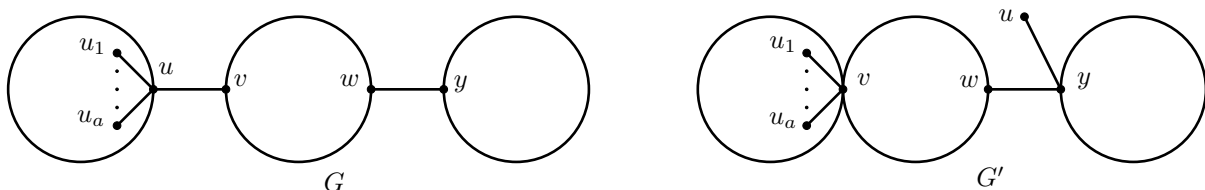


Figure 2.1: The graphs G' and G considered in Proposition 2.1.

Proof. Suppose that there are non-pendent cut edges uv and wy in G . Without loss of generality, we can assume that $d_G(u)d_G(v) \leq d_G(w)d_G(y)$ and the distance from u to y is greater than the distance from u to w . Clearly, the degrees of vertices u, v, w and y are greater than 1. For convenience, denote $d_G(u) = a+1$, $d_G(v) = b+1$ and $N_G(u) = \{v, u_1, u_2, \dots, u_a\}$.

Now we consider another graph G' , obtained from G , such that

$$G' = G - \{uv, uu_1, uu_2, \dots, uu_a\} + \{vu_1, vu_2, \dots, vu_a\} + uy$$

(see Figure 2.1). Then we have $d_{G'}(v) = a + b$, $d_{G'}(u) = 1$, $d_{G'}(y) = d_G(y) + 1$ and $d_{G'}(z) = d_G(z)$ for all $z \in V(G) \setminus \{u, v, y\}$. Also, it is easy to see that G' belongs to the class of graphs of order n with m edges and k cut edges. Therefore, by the definition of e^{M_2} , we have

$$\begin{aligned} e^{M_2}(G') - e^{M_2}(G) &= \sum_{i=1}^a e^{(a+b)d_G(u_i)} + \sum_{z \in N_G(v) \setminus \{u\}} e^{(a+b)d_G(z)} + \sum_{z \in N_G(y) \setminus \{w\}} e^{(d_G(y)+1)d_G(z)} + e^{d_G(w)(d_G(y)+1)} + e^{d_G(y)+1} \\ &\quad - \sum_{i=1}^a e^{(a+1)d_G(u_i)} - \sum_{z \in N_G(v) \setminus \{u\}} e^{(b+1)d_G(z)} - \sum_{z \in N_G(y) \setminus \{w\}} e^{d_G(y)d_G(z)} - e^{d_G(w)d_G(y)} - e^{d_G(u)d_G(v)} \\ &> e^{d_G(w)} e^{d_G(w)d_G(y)} - e^{d_G(w)d_G(y)} - e^{d_G(u)d_G(v)} > 0 \end{aligned}$$

since $a + b \geq a + 1$, $a + b \geq b + 1$, $e^{d_G(w)} > 2$ and $d_G(w)d_G(y) \geq d_G(u)d_G(v)$. This contradicts the fact that $e^{M_2}(G)$ is maximal in the class of graphs of order n with m edges and k cut edges. This completes the proof. $\square$

A tree with exactly two non-pendent vertices is called a double star. If the degrees of non-pendent vertices are a and b then the double star is denoted by $S_{a,b}$, where $a \geq b \geq 2$. When $b = 1$, we define $S_{a,1}$ to be the same as the star S_{a+1} . From the above proposition, the following two corollaries follow immediately.

Corollary 2.1. *Let G be a graph of order n with k cut edges. If $e^{M_2}(G)$ is maximum in $\mathcal{G}_n^{(k)}$, then the number of non-pendent cut edges of G is at most one.*

Corollary 2.2. [15, 16] *Let T be a tree of order n that maximizes e^{M_2} . Then T is isomorphic to the balanced double star $S_{\lceil n/2 \rceil, \lfloor n/2 \rfloor}$.*

Proof. The number of non-pendent cut edges in T is at most one by Proposition 2.1. Hence, there are at least $n - 2$ pendent edges in T . Therefore, we have $T \cong S_{a,b}$, where $a + b = n$ and $a \geq b \geq 1$.

Let $a - b \geq 2$. Then $ab \leq (n^2 - 4)/4$. From the definition of e^{M_2} , we have

$$e^{M_2}(T) = e^{ab} + (a - 1)e^a + (b - 1)e^b = e^{b(n-b)} + (n - b - 1)e^{n-b} + (b - 1)e^b.$$

Now we consider a function $f(t) = e^{t(n-t)} + (n - t - 1)e^{n-t} + (t - 1)e^t$ on $2 \leq t \leq \lfloor n/2 \rfloor$. Then

$$\begin{aligned} f'(t) &= (n - 2t)e^{t(n-t)} - (n - t)e^{n-t} + te^t = (n - t)e^{n-t} \left(\frac{n - 2t}{n - t} e^{(t-1)(n-t)} - 1 \right) + te^t \\ &\geq (n - t)e^{n-t} \left(\frac{n - 2t}{n - t} e^{n-2} - 1 \right) + te^t > (n - t)e^{n-t} \left(\frac{(n - 2t)(n - 1)}{n - t} - 1 \right) + te^t \\ &= e^{n-t}(n^2 - 2nt - 2n + 3t) + te^t > n^2 - 2nt - 2n + 3t + t(1 + t) = (n - 2t)(n - 2) + t^2 > 0 \end{aligned}$$

since $n \geq 2t \geq 4$ and $e^\alpha > 1 + \alpha$. Hence, $f(t)$ is increasing on $2 \leq t \leq \lfloor n/2 \rfloor$ and we get

$$e^{M_2}(T) = e^{b(n-b)} + (n - b - 1)e^{n-b} + (b - 1)e^b = f(b) \leq f(\lfloor n/2 \rfloor) = e^{M_2}(S_{\lceil n/2 \rceil, \lfloor n/2 \rfloor}).$$

This completes the proof. $\square$

If $k = n - 1$ then all graphs in $\mathcal{G}_n^{(k)}$ are trees of order n , and the extremal trees maximizing e^{M_2} were determined in the previous corollary. Additionally, the extremal graphs with maximum e^{M_2} in $\mathcal{G}_n^{(k)}$ are easily characterized for $k = 0$ and $k = 1$. Therefore, we may assume that $2 \leq k \leq n - 3$. Consequently, it follows that $n \geq 5$.

Theorem 2.2. *Let $e^{M_2}(G)$ be maximum in $\mathcal{G}_n^{(k)}$.*

(i) *If $g(0) < g(\lfloor k/2 \rfloor)$ then $G \cong G(\lceil k/2 \rceil, \lfloor k/2 \rfloor, 0, \dots, 0)$, where 0 occurs $n - k - 2$ times.*

(ii) *If $g(0) > g(\lfloor k/2 \rfloor)$ then $G \cong G(k, 0, 0, \dots, 0)$, where 0 occurs $n - k - 1$ times.*

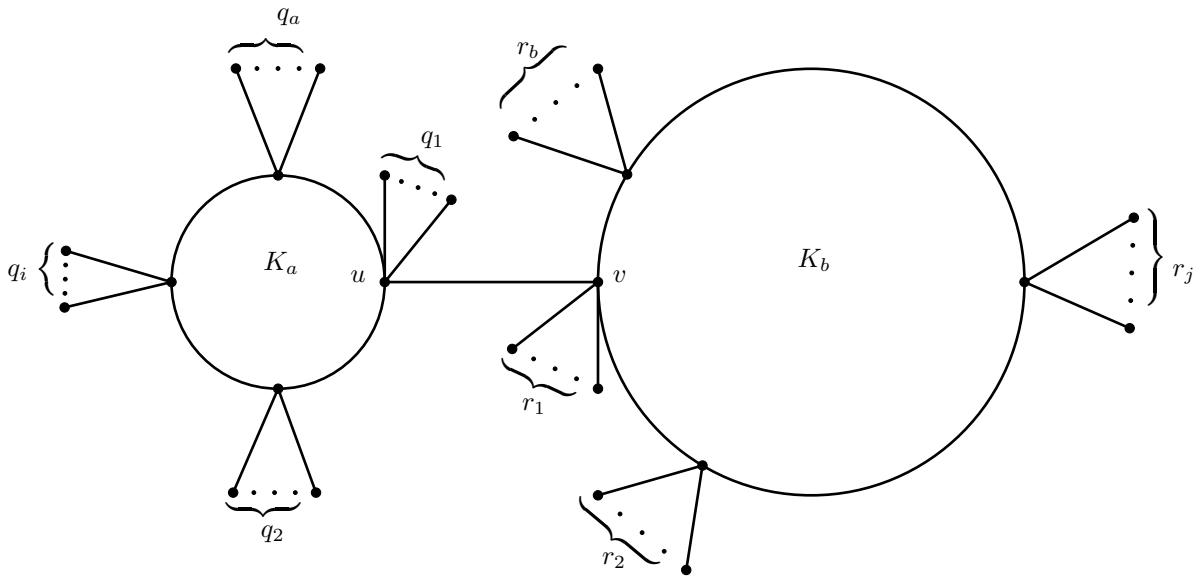


Figure 2.2: The graph $G(q_1, q_2, \dots, q_a) \cup G(r_1, r_2, \dots, r_b) + \{uv\}$.

Proof. If all cut edges in G are pendent, then $G \in \mathcal{G}_n^k$, and by Theorem 2.1, we obtain the required result. From Corollary 2.1, it follows that there is at most one non-pendent cut edge in G . Suppose there is exactly one non-pendent cut edge in G . Then one can easily see that

$$G \cong G(q_1, q_2, \dots, q_a) \cup G(r_1, r_2, \dots, r_b) + \{uv\},$$

where u is the vertex in $G(q_1, q_2, \dots, q_a)$ with respect to q_1 , v is the vertex in $G(r_1, r_2, \dots, r_b)$ with respect to r_1 ,

$$\sum_{i=1}^a q_i + \sum_{j=1}^b r_j = k - 1,$$

$a \geq 1$, $b \geq 1$ and $a + b = n - k + 1$ (see Figure 2.2). Since uv is the non-pendent cut edge in G , we have $d_G(u) \geq 2$ and $d_G(v) \geq 2$.

Claim: $\max_{xy \in E(G)} \{d_G(x)d_G(y)\} = d_G(v)d_G(u)$.

Proof of claim. Let wz be an edge in G such that $d_G(u)d_G(v) < d_G(w)d_G(z)$. Without loss of generality, we assume that $wz \in E(G(q_1, q_2, \dots, q_a))$ and $d_G(w) \geq 2$ since $4 \leq d_G(u)d_G(v) < d_G(w)d_G(z)$. Now we consider a graph

$$G_1 = G - \{vv_i \mid v_i \in N_G(v) \setminus \{u\}\} + \{wv_i \mid v_i \in N_G(v) \setminus \{u\}\}.$$

Then $d_{G_1}(w) = d_G(w) + d_G(v) - 1 \geq d_G(w) + 1$, $d_{G_1}(v) = 1$ and $d_{G_1}(x) = d_G(x)$ for all $x \in V(G) \setminus \{w, v\}$. Also, we have $G_1 \in \mathcal{G}_n^{(k)}$. From the definition of e^{M_2} , we obtain

$$\begin{aligned} e^{M_2}(G_1) - e^{M_2}(G) &= \sum_{x \in N_G(v) \setminus \{u\}} e^{(d_G(w)+d_G(v)-1)d_G(x)} + e^{d_G(u)} + \sum_{x \in N_G(w) \setminus \{z\}} e^{(d_G(w)+d_G(v)-1)d_G(x)} + e^{(d_G(w)+d_G(v)-1)d_G(z)} \\ &\quad - \sum_{x \in N_G(v) \setminus \{u\}} e^{d_G(v)d_G(x)} - e^{d_G(u)d_G(v)} - \sum_{x \in N_G(w) \setminus \{z\}} e^{d_G(w)d_G(x)} - e^{d_G(w)d_G(z)} \\ &> e^{(d_G(w)+1)d_G(z)} - e^{d_G(u)d_G(v)} - e^{d_G(w)d_G(z)} \\ &= e^{d_G(z)} \cdot e^{d_G(w)d_G(z)} - e^{d_G(u)d_G(v)} - e^{d_G(w)d_G(z)} \\ &> 2e^{d_G(w)d_G(z)} - e^{d_G(u)d_G(v)} - e^{d_G(w)d_G(z)} > 0 \end{aligned}$$

since $d_G(w) + d_G(v) - 1 > d_G(v)$, $e^{d_G(u)} > 0$, $d_G(w) + d_G(v) - 1 > d_G(w) + 1 > d_G(w)$ and $e^{d_G(z)} > 2$. This contradicts the fact that $e^{M_2}(G)$ is maximum in $\mathcal{G}_n^{(k)}$. The proof of the claim is finished.

We note that

$$d_G(u)d_G(v) = (a + q_1)(b + r_1) \leq \frac{(a + b + q_1 + r_1)^2}{4} \leq \frac{(n - k + 1 + k - 1)^2}{4} = \frac{n^2}{4}.$$

From the claim and the above inequality, we have

$$\begin{aligned} e^{M_2}(G) &= \sum_{xy \in E(G)} e^{d_G(x)d_G(y)} \leq \sum_{xy \in E(G)} e^{d_G(u)d_G(v)} = \left(\binom{a}{2} + \binom{b}{2} + k \right) e^{d_G(u)d_G(v)} \\ &\leq \frac{a^2 + b^2 - (a + b) + 2k}{2} \cdot e^{n^2/4} \leq \frac{a^2 + b^2 - (a + b) + 2(a - 1)(b - 1) + 2k}{2} \cdot e^{n^2/4} \\ &= \frac{(a + b - 1)^2 - (a + b - 1) + 2k}{2} \cdot e^{n^2/4} = \frac{(n - k)^2 - n + 3k}{2} \cdot e^{n^2/4}. \end{aligned} \quad (2)$$

Now we prove that

$$(n - k)^2 - n + 3k \leq 4 \left[(n - 1)^2 - (n - 1)k + \frac{k^2 - 1}{4} - \frac{n^2}{4} \right]. \quad (3)$$

It is equivalent to the following inequality

$$k(2n - 1) \leq (n - 3)(2n - 1),$$

and it holds for $k \leq n - 3$. From (2) and (3), we obtain

$$\begin{aligned} e^{M_2}(G) &\leq \frac{(n - k)^2 - n + 3k}{2} \cdot e^{\frac{n^2}{4}} \\ &\leq 2 \left[(n - 1)^2 - (n - 1)k + \frac{k^2 - 1}{4} - \frac{n^2}{4} \right] \cdot e^{\frac{n^2}{4}} \\ &\leq e^{(n-1)^2 - (n-1)k + \frac{k^2-1}{4} - \frac{n^2}{4}} \cdot e^{\frac{n^2}{4}} = e^{(n-1)^2 - (n-1)k + \frac{k^2-1}{4}} \\ &\leq e^{(n-1)^2 - (n-1)k + \lfloor \frac{k}{2} \rfloor \lceil \frac{k}{2} \rceil} = e^{(n - \lfloor \frac{k}{2} \rfloor - 1)(n - \lceil \frac{k}{2} \rceil - 1)} < e^{M_2}(G(\lceil k/2 \rceil, \lfloor k/2 \rfloor, \underbrace{0, \dots, 0}_{n-k-2})), \end{aligned}$$

since $2x < e^x$ for all positive integer x . This is a contradiction to the fact that $e^{M_2}(G)$ is maximum in $\mathcal{G}_n^{(k)}$, because $G(\lceil k/2 \rceil, \lfloor k/2 \rfloor, \underbrace{0, \dots, 0}_{n-k-2}) \in \mathcal{G}_n^{(k)}$. Hence, all cut edges in G are pendent, and the result follows directly from Theorem 2.1. $\square$

3. Graphs with the minimum exponential second Zagreb index

In this section, we study non-star graphs and determine the ones that attain the minimum exponential second Zagreb index.

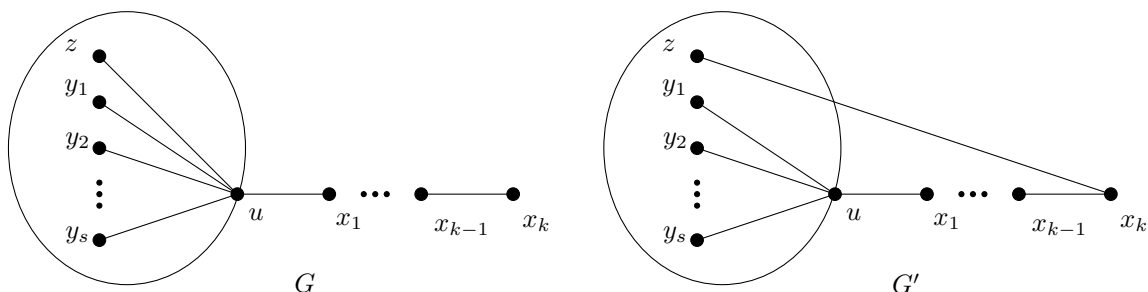


Figure 3.1: The transformation in Lemma 3.1.

Lemma 3.1. Let $ux_1 \cdots x_k$ be a pendent path in a connected graph G and z be a neighbor vertex of u such that $d_G(z) < 3$ and $z \neq x_1$. If $G' = G - uz + zx_k$ then $e^{M_2}(G) > e^{M_2}(G')$ (see Figure 3.1).

Proof. Clearly $d_G(v) = d_{G'}(v)$ for all $v \in V(G)$ such that $v \neq u$ and $v \neq x_k$. Let $N_G(u) = \{y_1, y_2, \dots, y_s, x_1, z\}$. Then $d_G(u) = s + 2 \geq 3$, $d_G(x_k) = 1$, $d_{G'}(u) = s + 1$ and $d_{G'}(x_k) = 2$.

Case (i). Let $k = 1$. Then there is a vertex y_j such that $d_G(y_j) \geq 2$ since G is different from the star. Hence, we have

$$\begin{aligned} e^{M_2}(G) - e^{M_2}(G') &= \sum_{i=1}^s e^{(s+2)d_G(y_i)} - \sum_{i=1}^s e^{(s+1)d_G(y_i)} + e^{s+2} - e^{(s+1) \cdot 2} + e^{(s+2)d_G(z)} - e^{2d_G(z)} \\ &\geq e^{(s+2)d_G(y_j)} - e^{(s+1)d_G(y_j)} - e^{(s+1) \cdot 2} > 0 \end{aligned}$$

since $s \geq 1$ and $d_G(y_j) \geq 2$.

Case (ii). Let $k \geq 2$. Then, we obtain

$$\begin{aligned} e^{M_2}(G) - e^{M_2}(G') &= \sum_{i=1}^s e^{(s+2)d_G(y_i)} - \sum_{i=1}^s e^{(s+1)d_G(y_i)} + e^{(s+2) \cdot 2} - e^{(s+1) \cdot 2} + e^{(s+2)d_G(z)} - e^{2d_G(z)} + e^{2 \cdot 1} - e^{2 \cdot 2} \\ &> e^{2s+2}(e^2 - 1) + e^{3d_G(z)} - e^4 + e^2 - e^4 \\ &> 3e^{2s+2} + e^{3d_G(z)} - e^4 + e^2 - e^4 \\ &> 3e^4 + e^{3d_G(z)} - e^4 + e^2 - e^4 > 0 \end{aligned}$$

since $s \geq 1$ and $d_G(z) < 3$. □

Lemma 3.2. Let P and Q be two pendent paths with origins u and v in graph G , respectively. Let x be a neighbor vertex of u on P and y be the pendent vertex on Q . If $d_G(u) \geq d_G(v)$ and $G' = G - ux + xy$ then $e^{M_2}(G) > e^{M_2}(G')$.

Proof. If $u = v$ then we easily get the required result by Lemma 3.1. Hence, suppose that $u \neq v$. Let $N_G(u) = \{x, u_1, u_2, \dots, u_s\}$ and $N_G(v) = \{y_1\}$. Then $d_G(u) = s + 1 \geq 3$ because u is the origin of P . Clearly $d_G(w) = d_{G'}(w)$ for all $w \in V(G)$ such that $w \neq u$ and $w \neq y$. Also, we may assume that $d_G(u_i) \geq 2$ for all $i = 1, 2, \dots, s$. Because, if $d_G(u_i) = 1$ then P and uu_i are two pendent paths with origin u . Therefore, we obtain

$$\begin{aligned} e^{M_2}(G) - e^{M_2}(G') &= \sum_{i=1}^s e^{(s+1)d_G(u_i)} + e^{(s+1)d_G(x)} + e^{d_G(y_1) \cdot 1} - \sum_{i=1}^s e^{sd_G(u_i)} - e^{2d_G(x)} - e^{d_G(y_1) \cdot 2} \\ &> \sum_{i=1}^s e^{sd_G(u_i)} (e^{d_G(u_i)} - 1) - e^{2d_G(y_1)} \\ &> se^{2s} \cdot 6 - e^{2d_G(v)} \geq 12e^{2s} - e^{2d_G(v)} \\ &> e^{2s+2} - e^{2d_G(v)} = e^{2d_G(u)} - e^{2d_G(v)} \geq 0, \end{aligned}$$

since $e^{(s+1)d_G(x)} > e^{2d_G(x)}$, $e^{d_G(y_1)} > 0$, $d_G(u_i) \geq 2$ ($i = 1, 2, \dots, s$) and $6s \geq 12 > e^2$. □

A star-like tree is a tree with exactly one vertex of degree greater than 2. In [4], it was proved that $e^{M_2}(T) > e^{M_2}(P_n)$ for any tree T of order n different from P_n .

Theorem 3.1. Let G be a connected graph of order n with maximum degree Δ , $3 \leq \Delta \leq n - 2$. Then

$$e^{M_2}(G) \geq e^{2\Delta} + (\Delta - 1)e^\Delta + (n - \Delta - 2)e^4 + e^2$$

with equality holding if and only if G is isomorphic to a star-like tree with maximum degree Δ in which exactly one neighbor of maximum degree vertex has degree two.

Proof. Let G be a graph with minimum $e^{M_2}(G)$ in the class of graphs with order n with maximum degree Δ . Also let w be a maximum degree vertex in G . If there is a non-cut edge xy in G that is not incident to w , then $e^{M_2}(G) > e^{M_2}(G - xy)$ and it follows that G is a tree. If there is a pendent path with origin $u \neq w$, then we easily get a contradiction by Lemma 3.2. Hence G is a star-like tree of order n with maximum degree Δ . Let s be the number of pendent vertices adjacent to w . Since $\Delta \leq n - 2$, we have $s \leq \Delta - 1$. Then

$$\begin{aligned} e^{M_2}(G) &= (\Delta - s)e^{2\Delta} + se^\Delta + (n - 1 - 2\Delta + s)e^4 + (\Delta - s)e^2 \\ &= s(e^\Delta + e^4 - e^{2\Delta} - e^2) + \Delta e^{2\Delta} + (n - 1 - 2\Delta)e^4 + \Delta e^2 \\ &\geq (\Delta - 1)(e^\Delta + e^4 - e^{2\Delta} - e^2) + \Delta e^{2\Delta} + (n - 1 - 2\Delta)e^4 + \Delta e^2 \\ &= e^{2\Delta} + (\Delta - 1)e^\Delta + (n - \Delta - 2)e^4 + e^2 \end{aligned}$$

since $e^\Delta + e^4 - e^{2\Delta} - e^2 < e^\Delta + e^4 - e^{\Delta+2} < e^\Delta + e^4 - 2e^{\Delta+1} < 0$. The equality holds if and only if G is a star-like tree and $s = \Delta - 1$. □

Theorem 3.2. *If $e^{M_2}(G)$ is minimum in the class of cyclic graphs of order n with girth g , such that $g \leq n - 1$, then G is isomorphic to the unicyclic graph that has exactly one pendent path of length $n - g$.*

Proof. Let C be a cycle of length g in G . If there is a non-cut edge $xy \notin C$ then $e^{M_2}(G) > e^{M_2}(G - xy)$ and it contradicts the fact that $e^{M_2}(G)$ is minimum. Hence we have G is unicyclic. Also, there is exactly one pendent path in G by Lemma 3.2. $\square$

Let $\mathcal{G}_n^{(k+)}$ be the class of cyclic graphs of order n with at least k , $k \leq n - 3$ cut edges. Then clearly, $\mathcal{G}_n^{(k)} \subseteq \mathcal{G}_n^{(k+)}$. Let U_n^g be the unicyclic graph of order n with girth g and exactly one pendent path of length $n - g$.

Theorem 3.3. *Let $e^{M_2}(G)$ be minimum in $\mathcal{G}_n^{(k+)}$.*

(i) *If $k = 0$ then $G \cong C_n$.*

(i) *If $k = 1$ then $G \cong U_n^{n-1}$.*

(ii) *If $k \geq 2$ then $G \in \{U_n^g \mid 3 \leq g \leq n - k\}$.*

Proof. Let g be the girth of G and C be a cycle of length g in G . Then $3 \leq g \leq n - k$ since $G \in \mathcal{G}_n^{(k+)}$. If there is a non-cut edge $xy \notin C$ then $e^{M_2}(G) > e^{M_2}(G - xy)$ and it contradicts the fact that $e^{M_2}(G)$ is minimum. Hence G is unicyclic with girth g . Also, there is exactly one pendent path in G by Lemma 3.2. Therefore, we have $G \in \{U_n^g \mid 3 \leq g \leq n - k\}$. If $k = 0$ then $C_n \in \{U_n^g \mid 3 \leq g \leq n - k\}$. If $k = 1$ then $U_n^{n-1} \in \{U_n^g \mid 3 \leq g \leq n - k\}$. Also, we have

$$e^{M_2}(C_n) < e^{M_2}(U_n^{n-1}) < e^{M_2}(U_n^{n-2}) = e^{M_2}(U_n^{n-4}) = \dots = e^{M_2}(U_n^3).$$

Hence, we obtain the required conclusions. $\square$

Theorem 3.4. *Let $G \in \mathcal{G}_n^{(k)}$. If $e^{M_2}(G)$ is minimum in $\mathcal{G}_n^{(k)}$, then $G \cong U_n^g$.*

Proof. Since $\mathcal{G}_n^{(k)} \subseteq \mathcal{G}_n^{(k+)}$ and $\mathcal{G}_n^{(k)} \cap \{U_n^g \mid 3 \leq g \leq n - k\} = \{U_n^g\}$, the required conclusion follows from Theorem 3.3. $\square$

Acknowledgment

The first author (B. Horoldagva) gratefully acknowledges the support provided by the Mongolian National University of Education (Funder ID: 100020678, Grant No. MNUE2025F023).

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