

An Open Problem on the Exponential of the Second Zagreb Index*

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Abstract

The second Zagreb index is $M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v)$. It was found to occur in certain approximate expressions of the total π -electron energy of alternant hydrocarbons and used by various researchers in their QSPR and QSAR studies. Recently the exponential of a vertex-degree-based topological index was introduced. It is known that among all trees with n vertices, the exponential of the second Zagreb index e^{M_2} attains its minimum value in the path P_n . In this paper, we show that e^{M_2} attains its maximum value in the balanced double star with n vertices and solve an open problem proposed by Cruz and Rada [R. Cruz, J. Rada, The path and the star as extremal values of vertex-degree-based topological indices among trees, MATCH Commun. Math. Comput. Chem. 82 (2019) 715-732].

1 Introduction

The first Zagreb index M_1 and the second Zagreb index M_2 were introduced 50 years ago [10]. The Zagreb indices and their variants have been used to study molecular complexity, chirality, ZE-isomerism and heterosystems whilst the overall Zagreb indices exhibited a potential applicability for deriving multilinear regression models. Zagreb indices are also used by various researchers in their QSPR and QSAR studies. Mathematical properties of the Zagreb indices have also been studied. Readers can refer to the paper [12] and the cited literature. The second Zagreb index was found to occur in certain approximate expressions of the total π -electron energy of alternant hydrocarbons [10]. We encourage the reader

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to consult [1, 4–8, 11, 15] for the historical background, computational techniques, and mathematical properties of the second Zagreb index.

For simple graph G with edge set $E(G)$, the second Zagreb index of G is defined as

$$M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v)$$

where $d_G(v)$ is the degree of the vertex v in G . It is a vertex-degree-based (VDB for short) topological index, also referred as bond incident degree index.

A formal definition of a VDB topological index is as follows. Let \mathcal{G}_n be the set of graphs with n non-isolated vertices. Consider the set

$$K = \{(i, j) \in \mathbf{N} \times \mathbf{N} : 1 \leq i \leq j \leq n - 1\}$$

and for a graph $G \in \mathcal{G}_n$, denote by $m_{i,j}(G)$ the number of edges in G joining vertices of degree i and j . A VDB topological index over \mathcal{G}_n is a function $\varphi : \mathcal{G}_n \rightarrow \mathbf{R}$ induced by real numbers $\{\varphi_{i,j}\}_{(i,j) \in K}$ defined as

$$\varphi(G) = \sum_{(i,j) \in K} m_{i,j}(G)\varphi_{i,j}$$

for every $G \in \mathcal{G}_n$.

Many important topological indices are obtained from different choices of $\varphi_{i,j}$. For example, the first Zagreb index M_1 induced by numbers $\varphi_{i,j} = i + j$; the second Zagreb index M_2 induced by $\varphi_{i,j} = ij$; the Randić index χ induced by $\varphi_{i,j} = \frac{1}{\sqrt{ij}}$, et al. For details on VDB topological indices, see [3, 9, 13, 14].

In order to study of the discrimination ability of topological indices, Rada [13] introduced the exponential of a vertex-degree-based topological index. Given a vertex-degree-based topological index φ , the exponential of φ , denoted by e^φ , is defined as

$$e^\varphi(G) = \sum_{(i,j) \in K} m_{i,j}(G)e^{\varphi_{i,j}}$$

The extremal value problem of e^φ over the set \mathcal{T}_n of trees with n vertices was initiated in [3], and it was shown that e^{M_1} , e^{M_2} attain their minimum value in the path P_n , e^χ , e^H , e^{GA} , e^{SC} , e^{AZ} attain their minimum value in the star S_n , e^{M_1} , e^{ABC} attain their maximum value in the star S_n , e^H , e^{GA} , e^{SC} attain their maximum value in the path P_n . In [2], it was shown that e^χ attains its maximum value in the path P_n . These results are summarized in Table 1.

Table 1. Results on extremal trees for exponential of well known VDB topological indices.

	e^{M_1}	e^{M_2}	e^X	e^H	e^{GA}	e^{SC}	e^{ABC}	e^{AZ}
min	P_n	P_n	S_n	S_n	S_n	S_n	?	S_n
max	S_n	?	P_n	P_n	P_n	P_n	S_n	?

The maximum value of e^{M_2} over \mathcal{T}_n is still an open problem. In this paper, we prove that the maximum value of e^{M_2} over \mathcal{T}_n is attained in the balanced double star $S_{\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil}$, and solve an open problem proposed by Cruz and Rada [3].

2 Trees with maximum exponential second Zagreb index

We first show in this section that in a maximal tree with respect to e^{M_2} over \mathcal{T}_n , the distance between any pendant vertex and any vertex with the maximum degree in T is at most 2

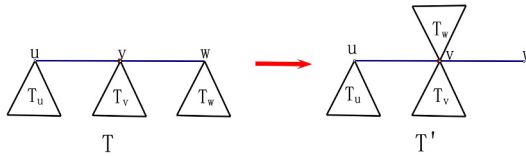


Figure 1. Trees T and T' in Lemma 1.

Lemma 1. *If T is a maximal tree with respect to e^{M_2} in \mathcal{T}_n , then the distance between a pendant vertex and a vertex with the maximum degree in T is at most 2.*

Proof. Otherwise, there is a vertex u with the maximum degree in T and a path $P = uvw$ such that w is not a pendant vertex in T . Let T_u, T_v and T_w be the components of $T - \{uv, vw\}$ containing u, v and w , respectively, see Figure 1. Let $d(u) = \Delta, d(v) = s, d(w) = t$, where $\Delta \geq s \geq 2, \Delta \geq t \geq 2$. The set of neighbours of v in T is $N_T(v) = \{u, w, v_1, v_2, \dots, v_{s-2}\}$ with $d_T(v_i) = x_i$ ($i = 1, 2, \dots, s - 2$), and the set of neighbours of w is $N_T(w) = \{v, w_1, w_2, \dots, w_{t-1}\}$ with $d(w_j) = y_j$ ($j = 1, 2, \dots, t - 1$). Let $T' = T - \{ww_1, ww_2, \dots, ww_{t-1}\} + \{vw_1, vw_2, \dots, vw_{t-1}\}$, then $d_{T'}(u) = \Delta, d_{T'}(v) = s + t - 1,$

$d_{T'}(w) = 1$ and

$$\begin{aligned}
 e^{M_2}(T') - e^{M_2}(T) &= e^{\Delta(s+t-1)} + \sum_{i=1}^{s-2} e^{x_i(s+t-1)} + \sum_{j=1}^{t-1} e^{y_j(s+t-1)} \\
 &\quad + e^{s+t-1} - (e^{\Delta s} + \sum_{i=1}^{s-2} e^{x_i s} + \sum_{j=1}^{t-1} e^{y_j t} + e^{st}) \\
 &= (e^{\Delta(s+t-1)} - e^{\Delta s} - e^{st}) + \sum_{i=1}^{s-2} (e^{x_i(s+t-1)} - e^{x_i s}) \\
 &\quad + \sum_{j=1}^{t-1} (e^{y_j(s+t-1)} - e^{y_j t}) + e^{s+t-1} > 0
 \end{aligned}$$

So, $e^{M_2}(T') > e^{M_2}(T)$ and T is not a maximal tree with respect to e^{M_2} in \mathcal{T}_n . ■

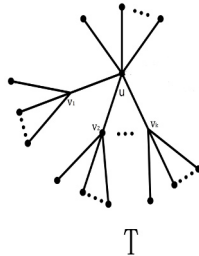


Figure 2. A tree T .

Remark. Let $T \in \mathcal{T}_n$ ($n \geq 4$), in which all distances between any pendant vertex and any vertex with the maximum degree are at most 2, then T has the form shown in Figure 2, where u is its unique vertex with the maximum degree if $k > 1$, or T is a double star if $k = 1$.

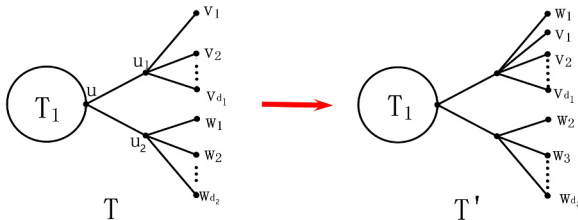


Figure 3. The trees T and T' in Lemma 2.

Lemma 2. Let T and T' be the trees on n vertices given in Figure 3, where u is a vertex with the maximum degree and T_1 is a subtree of T . If $d_1 \geq d_2 \geq 1$, then $e^{M_2}(T) < e^{M_2}(T')$.

Proof. Let $d_T(u) = \Delta$ be the maximum degree in T . The sets of neighbours of u_1 and u_2 in T are $N_T(u_1) = \{u, v_1, \dots, v_{d_1}\}$ and $N_T(u_2) = \{u, w_1, \dots, w_{d_2}\}$, respectively, where $d(v_1) = d(v_2) = \dots = d(v_{d_1}) = 1$, $d(w_1) = d(w_2) = \dots = d(w_{d_2}) = 1$. we assume that $d(u_1) \geq d(u_2)$. Let $T' = T - \{u_2w_1\} + \{u_1w_1\}$, then $d_{T'}(u_1) = d_1 + 2$, $d_{T'}(u_2) = d_2$, and

$$\begin{aligned} e^{M_2}(T') - e^{M_2}(T) &= e^{\Delta(d_1+2)} + (d_1 + 1)e^{(d_1+2)} + e^{\Delta d_2} + (d_2 - 1)e^{d_2} \\ &\quad - [e^{\Delta(d_1+1)} + d_1e^{(d_1+1)} + e^{\Delta(d_2+1)} + d_2e^{(d_2+1)}] \\ &= [e^{\Delta(d_1+1)} \cdot e^\Delta - e^{\Delta(d_1+1)}] + [d_1e^{(d_1+1)} \cdot e - d_1e^{(d_1+1)}] \\ &\quad + e^{(d_1+2)} + (e^{\Delta d_2} - e^{\Delta d_2} \cdot e^\Delta) + (d_2e^{d_2} - d_2e^{d_2} \cdot e) - e^{d_2} \\ &= [e^{\Delta(d_1+1)} - e^{\Delta d_2}][e^\Delta - 1] + [d_1e^{(d_1+1)} - d_2e^{d_2}](e - 1) \\ &\quad + [e^{(d_1+2)} - e^{d_2}] > 0 \end{aligned}$$

So, $e^{M_2}(T) < e^{M_2}(T')$. ■

In the following, we consider the double star $S_{x,y}$, it is a tree on $x + y + 2$ vertices with exactly two non-pendant vertices of degrees $x + 1$ and $y + 1$, respectively.

Lemma 3. *Let $T = S_{x,y}$ be the double star on n vertices, where $x + y = n - 2$. If T is a maximal tree with respect to e^{M_2} among all double stars on n vertices, then $|x - y| \leq 1$, i.e., T is the balanced double star with n vertices. And*

$$e^{M_2}(S_{\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil}) = \begin{cases} e^{\frac{n^2}{4}} + (n - 2)e^{\frac{n}{2}}, & \text{if } n \text{ is even;} \\ e^{\frac{n^2-1}{4}} + (\frac{n-3}{2})e^{\frac{n-1}{2}} + (\frac{n-1}{2})e^{\frac{n+1}{2}}, & \text{if } n \text{ is odd.} \end{cases}$$

Proof. Let u and v be two non-pendant vertices of the double star $T = S_{x,y}$, $d_T(u) = x + 1$ and $d_T(v) = y + 1$. Without loss of generality, we assume that $x \leq y$. If $|x - y| > 1$, let $T' = T - \{uv_1\} + \{uw_1\}$, where $v_1 \neq u$ is a neighbour of v in T , then $T' \simeq S_{x+1,y-1}$ and

$$\begin{aligned} e^{M_2}(T') - e^{M_2}(T) &= [e^{(x+2)y} + (x + 1)e^{(x+2)} + (y - 1)e^y] - [e^{(x+1)(y+1)} + xe^{x+1} + ye^{y+1}] \\ &= e^{(x+2)y} - e^{(x+1)(y+1)} - ye^{y+1} + (x + 1)e^{(x+2)} - xe^{x+1} + (y - 1)e^y \\ &> e^{xy+2y} - e^{xy+x+y+1} - ye^{y+1} = e^{xy+y}[e^y - e^{x+1}] - ye^{y+1} \\ &\geq e^{xy+y}[e^{x+2} - e^{x+1}] - ye^{y+1} = e^{xy+y+x+1}[e - 1] - ye^{y+1} \\ &> e^{xy+y+x+1} - ye^{y+1} = e^{y+1}[e^{x(y+1)} - y] > 0 \end{aligned}$$

So, $e^{M_2}(T') > e^{M_2}(T)$ and T is not maximal with respect to e^{M_2} among all double stars on n vertices. ■

Theorem 4. *If $T \in \mathcal{T}_n$ and $T \not\cong S_{\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil}$, $n \geq 4$, then T is not maximal with respect to e^{M_2} over \mathcal{T}_n .*

Proof. In fact, $e^{M_2}(S_{\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil}) > e^{M_2}(S_n)$ for $n \geq 4$, the star S_n on n vertices is not maximal with respect to e^{M_2} over \mathcal{T}_n .

If T is not a double star, then by Lemma 1, we may assume that all distances between a pendant vertex and a vertex with the maximum degree in T are at least 2 and T has the form depicted in Figure 2, where $k > 1$. By Lemma 2, T is not maximal.

So, T is a double star and the result follows from Lemma 3. ■

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