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An Exceptional Property of First Zagreb Index

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Abstract

The first Zagreb index is a molecular structure descriptor defined as $\sum_v \deg(v)^2$ where $\deg(v)$ is the degree (number of first neighbors) of the vertex v, and the summation embraces all vertices of the underlying molecular graph. We consider the generalized version of the first Zagreb index, defined as $\sum_v \deg(v)^p$, and show that for $p \geq 3$, its properties significantly differ from what is encountered in the case $p = 2$.

1 Introduction

The topological indices M_1 and M_2 belong among the oldest and most thoroughly examined graph–based molecular structure descriptors. They were introduced almost half a century ago [9, 10] and were eventually named "*first and second Zagreb group indices*" [1]; (later the word "*group*" was dropped from their names).

Let G be a graph whose vertex and edge sets are $V(G)$ and $E(G)$, respectively. Let $\deg(v)$ be the degree (= number of first neighbors) of the vertex $v \in V(G)$. Then

$$M_1 = M_1(G) = \sum_{v \in V(G)} \deg(v)^2$$

and

$$M_2 = M_2(G) = \sum_{uv \in E(G)} \deg(u)\,\deg(v)\ .$$

A vast amount of research on the Zagreb indices has been done so far. For details of their chemical applications and mathematical theory see the surveys [5,6,8,13] and the references cited therein. Yet, to the present author's best knowledge, the property of M_1 outlined in this paper has not been noticed until now.

The generalized version of the first Zagreb index, namely

$$Z_p = Z_p(G) = \sum_{v \in V(G)} \deg(v)^p ,$$

where p is some real number, seems to have been first considered by Li et al. [11,12]. In [11], the name "*first general Zagreb index* was proposed for Z_p.

Evidently, the ordinary Zagreb index M_1 is a special case of the general Zagreb index Z_p , for $p = 2$. It is less known that the case $p = 3$ was encountered in the early paper [10], but, for reasons not easy to understand, was ignored in all later considerations and applications of the Zagreb indices.

Let the graph G possess n vertices and m edges. In what follows, we assume that G is connected. Denote by n_k the number of vertices of G whose degree is equal to k. Then,

$$\sum_{k \geq 1} n_k = n \tag{1}$$

$$\sum_{k \geq 1} k \, n_k = 2m \tag{2}$$

$$\sum_{k \geq 1} k^2 \, n_k = M_1(G) \; . \tag{3}$$

In order to envisage the exceptional property of the first Zagreb index, we shall consider its generalized version Z_p , for which in analogy to Eq. (3) we have

$$Z_p(G) = \sum_{k \geq 1} k^p \, n_k \; . \tag{4}$$

2 A property of Z_p for $p \neq 2$

In what follows it will be assumed that the exponent p in Eq. (4) is a positive integer. In view of Eq. (2), the case $p = 1$ is trivial. Therefore, we shall examine Z_p for $p \geq 2$.

Multiply Eq. (1) by $2 \cdot 3^p$, multiply Eq. (2) by -3^p and add these to Eq. (4). This yields the identity

$$Z_p + 2 \cdot 3^p \, (n - m) = \sum_{k \geq 1} \Theta_p(k) \, n_k \tag{5}$$

where

$$\Theta_p(k) = k^p - 3^p \, k + 2 \cdot 3^p \ .$$

The term $\Theta_p(k)$ on the right–hand side of Eq. (5) is a polynomial of degree p in the variable k. This polynomial has a few noteworthy properties.

Property 1. If $k = 1$, then $\Theta_p(k) = 3^p + 1$. If $k = 2$, then $\Theta_p(k) = 2^p$. Thus, for $k = 1$ and $k = 2$, and for all $p \geq 2$, $\Theta_p(k)$ is positive–valued.

Property 2. If $k = 3$, then $\Theta_p(k) = 3^p - 3 \cdot 3^p + 2 \cdot 3^p = 0$. Thus, $k = 3$ is a root of the polynomial $\Theta_p(k)$ for all $p \geq 2$. In fact,

$$\Theta_p(k) = (k-3)\Big(k^{p-1} + 3\,k^{p-2} + 9\,k^{p-3} + \cdots + 3^{p-2}\,k + 3^{p-1} - 3^p\Big) \ .$$

Property 3. (a) If $p = 2$, then $\Theta_p(k) = k^2 - 9k + 18 = (k-3)(k-6)$. We see that $\Theta_2(k)$ is negative–valued for $k = 4$ and $k = 5$, zero for $k = 6$, and positive–valued for all $k \geq 7$.
(b) If $p = 3$, then $\Theta_p(k) = k^3 - 27k + 54 = (k-3)^2(k+6)$. Thus, $\Theta_3(k)$ is positive–valued for all $k \geq 4$.
(c) Also in the case $p \geq 4$, we have that $\Theta_p(k)$ is positive–valued for all $k \geq 4$.

In order to verify Property 3(c), note that

$$\frac{d\Theta_p(k)}{dk} = p\,k^{p-1} - 3^p$$

and that

$$p\,k^{p-1} - 3^p > 0$$

for $k \geq 4$ and $p \geq 4$. Therefore, $\Theta_p(k)$ monotonically increases, and since $\Theta_p(3) = 0$, it must be $\Theta_p(k) > 0$ for $k \geq 4$.

Combining Properties 1–3 we arrive at:

Property 4. (a) If $p \geq 3$, then all terms $\Theta_p(k)$, $k = 1, 2, 4, 5, 6, \ldots$ in Eq. (5) are greater than zero, whereas $\Theta_p(3) = 0$.
(b) Exceptionally, if $p = 2$, then some terms $\Theta_p(k)$ are negative–valued, namely those for $k = 4$ and $k = 5$.

The direct consequence of Property 4 is the following remarkable result:

Theorem 1. Let G be a (molecular) graph with n vertices, m edges, and n_ℓ vertices of degree ℓ , $\ell \neq 3$. Then for $p \geq 3$,

$$Z_p(G) \geq 2 \cdot 3^p \, (m - n) + \Theta_p(\ell) \, n_\ell \, .$$

Equality is attained if and only if all the remaining $n - n_\ell$ vertices of G are of degree 3. This equality case pertains to (n, m)-graphs with a fixed number of vertices of degree ℓ whose Z_p-value is minimal. The same graphs have minimal Z_p-values for all $p \geq 3$.

In what follows we focus our attention to the (chemically most relevant) special case of Theorem 1, for $\ell = 1$.

Theorem 2. Let G be a (molecular) graph with n vertices, m edges, and n_1 pendent vertices. Then for $p \geq 3$,

$$Z_p(G) \geq 2 \cdot 3^p \, (m - n) + (3^p + 1) \, n_1 \, .$$

Equality is attained if and only if all the remaining $n - n_1$ vertices of G are of degree 3. This equality case pertains to (n, m)-graphs with a fixed number of pendent vertices whose Z_p-value is minimal. The same graphs have minimal Z_p-values for all $p \geq 3$.

In Fig. 1 are depicted examples of trees ($m - n = -1$), unicyclic graphs ($m - n = 0$), and bicyclic graphs ($m - n = 1$) with 7 and 8 pendent vertices, whose Z_p-values are minimal.

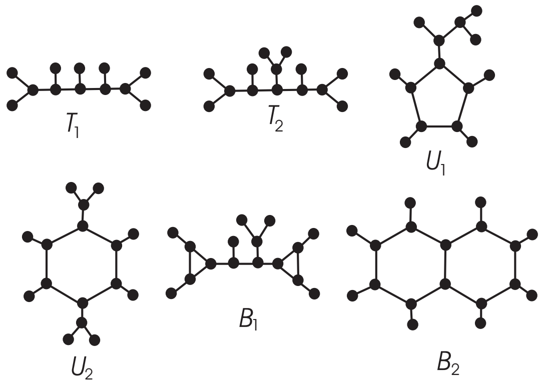

Fig. 1. Examples of trees (T_1, T_2), unicyclic graph (U_1, U_2), and bicyclic graphs (B_1, B_2) with 7 and 8 pendent vertices, having minimal Z_p-values for all $p \geq 3$, but not for $p = 2$.

Theorems 1 and 2 hold for all values of the exponent p, except for $p = 2$. In other words, Theorems 1 and 2 characterize the graphs with extremal general first Zagreb indices Z_p for any value of p, except that they do not characterize the graphs with extremal ordinary first Zagreb index.

As shown in the subsequent section, the case of $Z_2 \equiv M_1$ is significantly different, revealing that the original first Zagreb index, Eq. (3), is a kind of exception in the class of its generalized counterparts, Eq. (4).

3 A property of Z_p for $p = 2$

The solution of the problem for the case $p = 2$ was obtained by a lengthy trial-and-error guessing. However, after it was envisaged, it appears to be elementary:

Multiply Eq. (1) by 16, multiply Eq. (2) by -8 and add these to Eq. (3). This leads to the identity

$$M_1 + 16\,(n - m) = \sum_{k \geq 1} (k^2 + 16 - 8k)\, n_k = \sum_{k \geq 1} (k - 4)^2\, n_k \ . \tag{6}$$

Evidently, the multipliers $(k-4)^2$ on the right–hand side of Eq. (6) are positive–valued for all $k \neq 4$ and are equal to zero for $k = 4$. Therefore, in analogy to Theorems 1 and 2 we now have:

Theorem 3. Let G be a (molecular) graph with n vertices, m edges, and n_ℓ vertices of degree ℓ , $\ell \neq 4$. Then for $p = 2$,

$$Z_2(G) \equiv M_1(G) \geq 16(m-n) + (\ell-4)^2\, n_\ell \ .$$

Equality is attained if and only if all the remaining $n - n_\ell$ vertices of G are of degree 4 (provided that such graphs exist). This equality case pertains to (n, m)-graphs with a fixed number of vertices of degree ℓ whose first Zagreb indices are minimal.

Theorem 4. Let G be a (molecular) graph with n vertices, m edges, and n_1 pendent vertices. Then for $p = 2$,

$$Z_p(G) \equiv M_1(G) \geq 16(m-n) + 9\, n_1 \ .$$

Equality is attained if and only if the number of pendent vertices is even, and all the remaining $n - n_1$ vertices of G are of degree 4. This equality case pertains to (n, m)-graphs with a fixed number of pendent vertices whose first Zagreb indices are minimal.

In Fig. 2 are depicted examples of trees $(m - n = -1)$, unicyclic graphs $(m - n = 0)$, and bicyclic graphs $(m - n = 1)$ with 10 pendent vertices, whose first Zagreb indices are minimal.

The special case of Theorem 4 for trees was earlier reported by Goubko [2], who also characterized the trees with odd n_1 and minimal M_1-value (see also [7]). Analogous, but much more difficult results were obtained also for the second Zagreb index [2–4].

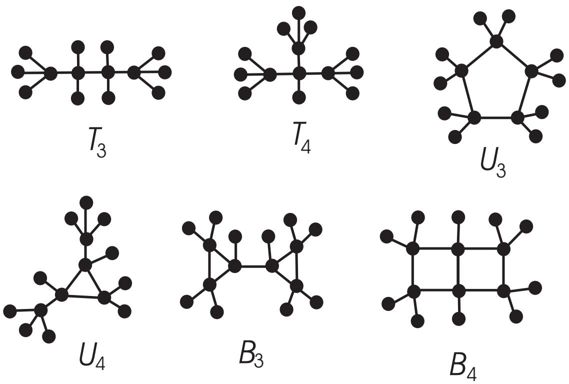

Fig. 2. Examples of trees (T_3, T_4), unicyclic graphs (U_3, U_4), and bicyclic graphs (B_3, B_4) with 10 pendent vertices, having minimal first Zagreb indices, but not minimal Z_p-values for $p > 2$.

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