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MULTIPLICATIVE ZAGREB INDICES OF TREES

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Abstract

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The first and second multiplicative Zagreb indices of G are $\Pi_1 = \prod_{x \in V(G)} \deg(x)^2$ and $\Pi_2 = \prod_{xy \in E(G)} deg(x) \deg(y)$, respectively, where $deg(v)$ is the degree of the vertex v. Let $\mathcal{T}_n$ be the set of trees with n vertices. We determine the elements of $\mathcal{T}_n$, extremal w.r.t. Π_1 and Π_2.

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1 Introduction

In this article we are concerned with simple graphs, that is finite and undirected graphs without loops and multiple edges. Let G be such a graph and $V(G)$ and $E(G)$ its vertex set and edge set, respectively. An edge of G, connecting the vertices x and y will be denoted by xy.

The degree $\deg(x)$ of a vertex $x \in V(G)$ is the number of vertices of G adjacent to x. A vertex of degree one is said to be pendent. A vertex adjacent to all other vertices is said to be fully connected.

A tree is a connected acyclic graph. The set of all n-vertex trees will be denoted by $\mathcal{T}_n$.

The n-vertex tree with a single fully connected vertex (and therefore with $n-1$ pendent vertices) is the star S_n. The n-vertex tree with exactly two pendent vertices is the path P_n.

The vertex–degree–based graph invariants

$$M_1(G) = \sum_{x \in V(G)} \deg(x)^2 \qquad \text{and} \qquad M_2(G) = \sum_{xy \in E(G)} deg(x) \deg(y)$$

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are known under the name first and second Zagreb index, respectively. They have been conceived in the 1970s and found considerable applications in chemistry [9, 12]. The Zagreb indices were subject to a large number of mathematical studies, of which we mention only a few newest [1, 2, 3, 6, 7, 13].

Todeschini et al. [10, 11] have recently proposed to consider the multiplicative variants of additive graph invariants, which applied to the Zagreb indices would lead to

$$\Pi_1 = \Pi(G) = \prod_{x \in V(G)} \deg(x)^2$$

and

$$\Pi_2 = \Pi_2(G) = \prod_{xy \in E(G)} deg(x) \deg(y) \ . \tag{1}$$

The properties of these "*multiplicative Zagreb indices*" have not been studied so far (but see below), and the present work is an attempt to contribute towards their better understanding.

In the 1980s, Narumi and Katayama [8] considered the product

$$NK = \prod_{x \in V(G)} \deg(x) \tag{2}$$

which nowadays in usually referred to as the "*Narumi–Katayama index*". Evidently, the first multiplicative Zagreb index is just the square of the Narumi–Katayama index, $\Pi_1 = (NK)^2$, and thus should not be viewed as something new.

In the recent works [4, 5], as well as in earlier works on the Narumi–Katayama index, the problem of finding graphs extremal w.r.t. NK was not considered at all.

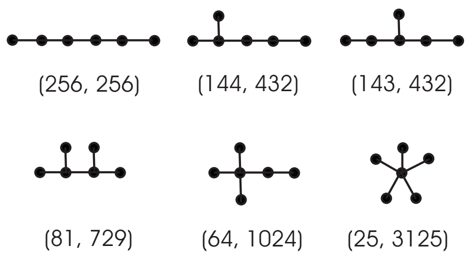

Figure 1: The 6-vertex trees and their (Π_1, Π_2)-values

In Fig. 1 are depicted all n-vertex trees for $n = 6$ and their Π_1- and Π_2-values indicated. This example (as well as analogous examples for other values of n) suggest the possibility that the following results hold:

Theorem 1.1 *Let $n \geq 5$ and let $T_n \in \mathcal{T}_n$, $T_n \ncong P_n, S_n$. Then*

$$\Pi_1(S_n) < \Pi_1(T_n) < \Pi_1(P_n) \tag{3}$$

$$\Pi_2(P_n) < \Pi_2(T_n) < \Pi_2(S_n) \ . \tag{4}$$

In Theorem 1.1, n cannot be less than five. Namely, for $n = 1, 2, 3$ the set $\mathcal{T}_n$ has just a single element, whereas for $n = 4$, $\mathcal{T}_n = \{S_n, P_n\}$.

In what follows we prove that Theorem 1.1 is indeed valid.

2 Proof of Inequalities (3)

For the sake of convenience, instead of $\Pi_1(G)$ we shall examine its logarithm, $L_1 = L_1(G) := \ln \Pi_1(G)$. Then,

$$L_1 = 2 \sum_{i=1}^{n-1} (\ln i)\, n_i \tag{5}$$

where n_i stands for the number of vertices of degree i .

Recall that for a graph with n vertices and m edges,

$$\sum_{i=1}^{n} n_i = n \tag{6}$$

$$\sum_{i=1}^{n} i\, n_i = 2m \tag{7}$$

and that for an n-vertex tree, $m = n - 1$.

Subtracting Eq. (6) from (7) we get (for trees)

$$n_2 = n - 2 - \sum_{i \geq 3} (i-1)\, n_i \tag{8}$$

which substituted back into (5) yields

$$L_1 = 2(n-2)\, \ln 2 - \sum_{i \geq 3} 2\, [(i-1)\, \ln 2 - \ln i]\, n_i \ . \tag{9}$$

Noting that

$$(i-1)\, \ln 2 - \ln i = \ln \frac{2^i}{2i}$$

we see that for $i \geq 3$ the multipliers in the summation on the right–hand side of Eq. (9) are positive-valued. Therefore, L_1 will attain its maximal value if $n_i = 0$ for all $i \geq 3$, i. e., if the underlying tree has no vertices of degree greater than two. The only tree satisfying this requirement is the path P_n . This proves the right–hand side of inequality (3).

In order to verify the validity of the left–hand side of (3), express from Eq. (6) the number of fully connected vertices (n_{n-1}), and substitute it back into (5). This yields:

$$L_1 = 2n\,\ln(n-1) - \sum_{i=1}^{n-2} 2\,[\ln(n-1) - \ln i]\, n_i \ .$$

Since $\ln(n-1) - \ln i$ is positive–valued and monotonically decreases with i, we see that L_1 will be minimal if the respective tree would have as many as possible pendent vertices, i. e., if this tree is the star.

This completes the proof of the inequalities (3). □

3 Proof of Inequalities (4)

We first need an auxiliary result:

Lemma 3.1 *The second multiplicative Zagreb index, defined via Eq. (1), can be written as*

$$\Pi_2(G) = \prod_{x \in V(G)} \deg(x)^{\deg(x)} \ .$$

Proof. The vertex x is the endpoint of $\deg(x)$ edges of G. Therefore in the product on the right–hand side of (1), the factor $\deg(x)$ occurs $\deg(x)$ times. □

Also here it is convenient to examine the logarithm of Π_2, which we denote by L_2. In view of Lemma 3.1,

$$L_2 = \sum_{i=1}^{n-1} (i\,\ln i)\, n_i \ . \tag{10}$$

We proceed in an analogous manner as in the previous section: By substituting Eq. (8) into (10), we get

$$L_2 = 2(n-2)\,\ln 2 + \sum_{i \geq 3} [i\,\ln i - (2\,\ln 2)(i-1)]\, n_i \ . \tag{11}$$

Claim 1. For $i \geq 3$, the multipliers in the summation on the right–hand side of Eq. (11) are positive–valued.

Proof. In order to verify Claim 1, note that

$$i\,\ln i - (2\,\ln 2)(i-1) = i(\ln i - \ln 4) + 2\,\ln 2$$

which evidently is greater than zero for $i \geq 4$. For $i = 3$, $i\,\ln i - (2\,\ln 2)(i-1) = \ln(27/16) > 0$. Thus, Claim 1 is true. □

Because of Eq. (11) and Claim 1, L_2 will be minimal if $n_i = 0$ holds for all $i \geq 3$. As we already know, the only tree obeying this requirement is the path

P_n . Hence, P_n is the tree with minimal second multiplicative Zagreb index, i. e., the left–hand side inequality in (4) holds.

In order to characterize the tree with maximal Π_2 , subtract Eq. (6) from (7), express n_{n-1} , and substitute back into (10). This yields:

$$L_2 = (n-1)\,\ln(n-1) - \sum_{2 \le i \le n-2} \left[\frac{(n-1)\,\ln(n-1)}{n-2} - \frac{i\,\ln i}{i-1} \right] (i-1)\, n_i \ . \tag{12}$$

Claim 2. For $2 \le i \le n-2$, the multipliers in the summation on the right–hand side of Eq. (12) are positive–valued.

Proof. It suffices to show that

$$\frac{(n-1)\,\ln(n-1)}{n-2} - \frac{i\,\ln i}{i-1} > 0 \ .$$

Consider the function $f(x) := (x\,\ln x)/(x-1)$. Its first derivative is equal to $(x-1-\ln x)/(x-1)^2$.

Now, for $x \ge 2$, $x-1-\ln x > 0$. To see this, note that

$$x - 1 - \ln x|_{x=1} = 0$$

and

$$(x-1-\ln x)' = 1 - 1/x$$

which for $x \ge 2$ is greater than zero. Therefore, for $x \ge 2$, $(x-1-\ln x)/(x-1)^2 > 0$, and $f(x)$ monotonically increases.

Next observe that

$$\left. \frac{(n-1)\,\ln(n-1)}{n-2} - \frac{i\,\ln i}{i-1} \right|_{i=n-1} = 0 \ .$$

Therefore, for $i < n-1$, this expression must be greater than zero. This implies Claim 2. □

In view of Eq. (12) and Claim 2, L_2 will be maximal if $n_i = 0$ for all $i = 2, \ldots, n-1$, i. e., if the underlying graph has only pendent and fully connected vertices. The unique tree in which all vertices are either pendent or fully connected is the star. Hence, the right–hand side inequality in (4) holds. □

4 The Second–Extremal Trees

Using an analogous, yet slightly more complicated, reasoning it is possible to characterize the trees that have second–minimal and second–maximal multiplicative Zagreb indices. We state these results without proof.

Let P_n^* be a tree (of the several possible) with exactly three pendent vertices. Let S_n^* be the graph obtained by inserting a new vertex (of degree two) to one of the edges of the star S_{n-1} . Then we have:

Theorem 4.1 *Let $n \geq 6$ and let $T_n \in \mathcal{T}_n$, $T_n \ncong P_n, S_n, P_n^*, S_n^*$. Then*

$$\Pi_1(S_n^*) < \Pi_1(T_n) < \Pi_1(P_n^*)$$

$$\Pi_2(P_n^*) < \Pi_2(T_n) < \Pi_2(S_n^*) \ .$$

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