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TREES WITH FIXED NUMBER OF PENDENT VERTICES WITH MINIMAL FIRST ZAGREB INDEX

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Abstract. The first Zagreb index M_1 of a graph G is equal to the sum of squares of the vertex degrees of G. In a recent work [Goubko, MATCH Commun. Math. Comput. Chem. **71** (2014), 33–46], it was shown that for a tree with n_1 pendent vertices, the inequality $M_1 \geqslant 9\,n_1 - 16$ holds. We now provide an alternative proof of this relation, and characterize the trees for which the equality holds.

1. Introduction

Throughout this paper we are concerned with simple graphs, that is graphs without multiple or directed edges, and without self-loops. Let G be such a graph, with vertex set $V(G)$. The degree $\deg(v)$ of a vertex $v \in V(G)$ is the number of vertices of G adjacent to v. The graph invariant M_1

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

has been previously much studied in the mathematical literature [**1**–**4**, **6**, **12**, **14**, **15**]. Its applications in chemistry are long known [**10**, **11**] and are nowadays well documented [**8**, **9**, **13**]. M_1 is nowadays referred to as the *first Zagreb index* of the graph G. A large number of results on M_1 has been obtained so far, most of which being inequalities (see [**5**, **15**–**18**] and the references cited therein).

One of the present authors [**7**] has recently established a remarkable inequality for the first Zagreb index of trees, relating M_1 with the number of pendent vertices, and only with this structural parameter.

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We now offer a different (simpler) proof of this result, which enables us to characterize the equality case. In particular, we now prove:

THEOREM 1.1. *Let T be a tree with n_1 pendent vertices and first Zagreb index $M_1(T)$. (a) If n_1 is even, then $M_1(T) \geqslant 9\,n_1 - 16$ with equality if and only if all non-pendent vertices of T are of degree 4. (b) If n_1 is odd, then $M_1(T) \geqslant 9\,n_1 - 15$ with equality if and only if all non-pendent vertices of T, except one, are of degree 4, and a single vertex of T is of degree 3 or 5.*

2. Proof of Theorem 1.1

Denote by n_k the number of vertices of degree k. Then, for a tree T with n vertices (and thus with $n-1$ edges),

$$\sum_{k \geqslant 1} n_k = n \tag{2.1}$$

$$\sum_{k \geqslant 1} k\, n_k = 2(n-1) \tag{2.2}$$

$$\sum_{k \geqslant 1} k^2\, n_k = M_1(T)\ .$$

Combining (2.1) and (2.2), we get

$$\sum_{k \geqslant 1} (k-2) n_k = -2\ . \tag{2.3}$$

Let g be a positive integer, different from 2. Then (2.3) can be rewritten as

$$(g-2) n_g + \sum_{k \neq g} (k-2) n_k = -2$$

i.e.,

$$n_g = \frac{1}{g-2} \left[-2 - \sum_{k \neq g} (k-2) n_k \right]. \tag{2.4}$$

Since

$$M_1(T) = g^2\, n_g + \sum_{k \neq g} k^2\, n_k$$

by using (2.4), we get

$$M_1(T) = -\frac{2\,g^2}{g-2} + \sum_{k \neq g} \left[k^2 - \frac{(k-2)g^2}{g-2} \right] n_k$$

and further

$$M_1(T) = \left(1 + \frac{g^2}{g-2} \right) n_1 - \frac{2\,g^2}{g-2} + \sum_{k \neq 1,g} \left[k^2 - \frac{(k-2)g^2}{g-2} \right] n_k\ . \tag{2.5}$$

The special case of formula (2.5), for $g = 4$ reads:

$$M_1(T) = 9\,n_1 - 16 + \sum_{k \neq 1,4} (k-4)^2\, n_k \ . \tag{2.6}$$

We shall return to Eq. (2.6) in a while.

Consider first Eq. (2.5) and the multipliers $k^2-(k-2)g^2/(g-2)$ in it. By direct calculation, we find that the equation $k^2-(k-2)g^2/(g-2)=0$ has two solutions: $2g/(g-2)$ and g. For k lying between these two values, $k^2-(k-2)g^2/(g-2)$ is negative–valued. By direct checking, we see that for all $g \geqslant 3$, except for $g = 4$, there exist some integer values of k for which $k^2-(k-2)g^2/(g-2) < 0$. Consequently, if $g \neq 4$, Eq. (2.5) is useless as far as the quest for trees with minimal M_1-value is concerned.

Eq. (2.6) has the advantage that in it all multipliers $(k-4)^2$ are positive–valued. Consequently, for a fixed n_1, its right–hand side will be minimal if $n_k = 0$ holds for all $k \neq 1, 4$. In other words, this must be trees with all non-pendent vertices of degree 4, provided such trees do exist.

A tree with all non-pendent vertices of degree 4 has $n_1 = 2(n_4 + 1)$ pendent vertices. Thus, if n_1 is even, part (a) of Theorem 1 follows.

A tree with odd n_1 must possess a non-pendent vertex of odd degree. From Eq. (2.6) we see that in order that the right–hand side of (2.6) be minimal, this must be either a single vertex of degree 3 or a single vertex of degree 5. Namely, only in these two cases will the term $\sum\limits_{k \neq 1,4} (k-4)^2\, n_k$ assume its smallest non-zero value, equal to unity. This implies part (b) of Theorem 1.

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