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GRAPHS WITH FIXED NUMBER OF PENDENT VERTICES AND 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 degrees of the vertices of G. Goubko proved that for trees with n_1 pendent vertices, $M_1 \geq 9\,n_1 - 16$. We show how this result can be extended to hold for any connected graph with cyclomatic number $\gamma \geq 0$. In addition, graphs with n vertices, n_1 pendent vertices, cyclomatic number γ, and minimal M_1 are characterized. Explicit expressions for minimal M_1 are given for $\gamma = 0, 1, 2$, which directly can be extended for $\gamma > 2$.

1. Introduction

In this paper we are concerned with simple connected graphs. Let G be such a graph and let its vertex set be $V(G)$. The number of vertices and edges of G are denoted by n and m, respectively. For connected graphs, the cyclomatic number (= number of independent cycles) is equal to $\gamma = m-n+1$. Recall that graphs with $\gamma = 0, 1, 2$ are referred to as trees, unicyclic graphs, and bicyclic graphs, respectively.

Let $\deg(v)$ be the degree (= number of first neighbors) of the vertex $v \in V(G)$. In the 1970 the graph invariant

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

has been considered in connection with certain chemical applications [10]. Eventually, it became known under the name *first Zagreb index*.

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A vast amount of research on the first Zagreb index has been done so far. For details of its mathematical theory see the surveys [7,8], the recent papers [1,3–6,9,11–13], and the references cited therein.

The number of vertices of degree k will be denoted by n_k . Then, evidently,

$$\sum_{k\geq 1} n_k = n, \tag{1.1}$$

$$\sum_{k\geq 1} k\, n_k = 2m, \tag{1.2}$$

and

$$\sum_{k\geq 1} k^2\, n_k = M_1(G). \tag{1.3}$$

If $deg(v) = 1$, then the vertex v is said to be pendent. Then n_1 is the number of pendent vertices, and the respective graph will be said to be an n_1-graph.

2. Goubko's theorem and its generalization

Recently, Goubko [4] discovered an interesting property of n_1-trees, namely that any n_1-tree T obeys the inequality $M_1(T) \geq 9\,n_1 - 16$, irrespective the number of its vertices (see also [5, 6, 9]). We now show that Goubko's theorem can be directly extended to any n_1-graph with a fixed value of cyclomatic number.

Theorem 2.1. *Let G be a connected graph with n_1 pendent vertices and cyclomatic number γ. Then*

$$M_1(G) \geq 9\,n_1 + 16(\gamma - 1). \tag{2.1}$$

Equality in (2.1) holds if and only if all non-pendent vertices of G are of degree 4, provided such graphs exist.

Proof. Multiply Eq. (1.1) by 16, multiply Eq. (1.2) by −8, and add these to Eq. (1.3). This yields

$$\sum_{k\geq 1}(k^2 + 16 - 8k)n_k = M_1 + 16(n - m) = M_1(G) - 16(\gamma - 1),$$

i.e.,

$$\begin{aligned} M_1(G) &= 16(\gamma - 1) + \sum_{k\geq 1}(k - 4)^2\, n_k \\ &= 16(\gamma - 1) + 9\,n_1 + \sum_{k\geq 2}(k - 4)^2\, n_k\,. \qquad (2.2) \end{aligned}$$

Theorem 2.1 is an immediate consequence of Eq. (2.2). □

Corollary 2.2. *If graphs, specified in Theorem 2.1, for which the equality* $M_1 = 9n_1 - 16(\gamma - 1)$ *holds, do not exist, then*

$$M_1(G) \geq 9\,n_1 + 16(\gamma - 1) + 1. \tag{2.3}$$

Equality in (2.3) holds if and only if one non-pendent vertex of G is of degree 3 and all other non-pendent vertices are of degree 4, and/or one non-pendent vertex of G is of degree 5 and all other non-pendent vertices are of degree 4, provided such graphs exist.

The original result of Goubko is just the special case of Theorem 2.1 and Corollary 2.2 for $\gamma = 0$.

Although Eq. (2.1) in Goubko's theorem 2.1 provides an elegant and simple structural condition for graphs with minimal first Zagreb indices, it is restricted to graphs with very special number of vertices. Thus, Goubko's theorem determines the n_1-trees and n_1-unicyclic graphs with minimal first Zagreb index only if $n = (3/2)n_1 - 1$ and $n = (3/2)n_1$, respectively, and requires that n_1 be even.

In what follows we show how this limitation can be circumvented. For this we need an auxiliary result [2, 14].

3. An auxiliary lemma

Let $i_1, i_2, \ldots, i_n$ be integers. We say that these integers are *almost equal* if

$$\max\Big\{i_1, i_2, \ldots, i_n\Big\} - \min\Big\{i_1, i_2, \ldots, i_n\Big\} \leq 1.$$

Lemma 3.1. [2, 14] *Let* $\mathcal{G}_{n,m}$ *be a class of graphs with n vertices and m edges. The first Zagreb index of a graph* $G \in \mathcal{G}_{n,m}$ *will be minimal if the degrees of its non-pendent vertices are almost equal, provided such a graph exists in* $\mathcal{G}_{n,m}$ *.*

Proof. Let u and v be any two vertices of the graph G. Let $\deg(u) = a$ and $\deg(v) = b$, such that $a - b = 2k$ or $2k + 1$, where k is non-negative integer. If G' is a graph obtained from G so that $\deg(u) = a - k$, $\deg(v) = b + k$ whereas the degrees of all other vertices in G' are same as in G, then

$$\begin{aligned} M_1(G) - M_1(G') &= a^2 + b^2 - \Big[(a-k)^2 + (b+k)^2\Big] \\ &= 2k(a-b-k) = \begin{cases} 2k^2 & \text{if } a - b = 2k, \\ 2k(k+1) & \text{if } a - b = 2k+1, \end{cases} \end{aligned}$$

implying $M_1(G) - M_1(G') \geq 0$, and that this difference is minimal for $k = 0$, i.e., if the degrees of u and v are almost equal. $\square$

4. (n, n_1)-Trees with minimal first Zagreb index

A graph with n vertices and n_1 pendent vertices will be said to be an (n, n_1)-graph. In the subsequent sections we characterize (n, n_1)-graphs with a given cyclomatic number, having minimal first Zagreb index. We begin with the case $\gamma = 0$.

Theorem 4.1. *Let T be a tree of order n with n_1 pendent vertices. Then*

$$M_1(T) \geq 4n - 6 + (n + n_1 - 4) \left\lfloor \frac{n-2}{n-n_1} \right\rfloor - (n - n_1) \left\lfloor \frac{n-2}{n-n_1} \right\rfloor^2 . \tag{4.1}$$

Equality in (4.1) is attained if and only if T consists of n_1 pendent vertices, $n_t = (n-n_1) \left\lfloor \frac{n-2}{n-n_1} \right\rfloor - n_1 + 2$ vertices of degree $t = \left\lfloor \frac{n-2}{n-n_1} \right\rfloor + 1$, and $n_{t+1} = n - 2 - (n - n_1) \left\lfloor \frac{n-2}{n-n_1} \right\rfloor$ vertices of degree $t + 1$.

Proof. Suppose that the tree T has minimal Zagreb index. Then by Lemma 3.1 it has n_t $(0 < n_t \leq n - n_1)$ non-pendent vertices of degree t and $n_{t+1} = n - n_1 - n_t$ non-pendent vertices of degree $t + 1$. Then,

$$M_1(T) = n_1 + n_t\, t^2 + n_{t+1}\, (t + 1)^2.$$

The parameters t, n_t, and n_{t+1} are calculated from the conditions

$$n_1 + n_t + n_{t+1} = n \tag{4.2}$$

$$n_1 + t\, n_t + (t + 1)n_{t+1} = 2m = 2(n - 1), \tag{4.3}$$

which yield

$$t(n - n_1) - n_t = n - 2 \qquad \text{i.e.,} \qquad t = \frac{n-2}{n-n_1} + \frac{n_t}{n-n_1}.$$

Since t is a positive integer, we get

$$t = \left\lfloor \frac{n-2}{n-n_1} \right\rfloor + 1,$$

which substituted back into Eqs. (4.2) and (4.3) leads to

$$\begin{aligned} n_t &= (n - n_1) \left\lfloor \frac{n-2}{n-n_1} \right\rfloor - n_1 + 2 \\ n_{t+1} &= n - 2 - (n - n_1) \left\lfloor \frac{n-2}{n-n_1} \right\rfloor , \end{aligned}$$

as required. □

(n, n_1)-Trees with minimal first Zagreb index, of the form specified in Theorem 4.1, exist for any value of n and n_1, provided $n > n_1 \geq 2$.

5. Unicyclic and bicyclic (n, n_1)-graphs with minimal first Zagreb index

If $\gamma > 0$ the considerations are fully analogous. Instead of Eq. (4.3) one has to use

$$n_1 + t\, n_t + (t+1)n_{t+1} = 2m = 2(n - 1 + \gamma), \tag{5.1}$$

assuming that graphs with the required degree distribution do exist. Without proof we state the results for $\gamma = 1$ and $\gamma = 2$.

Theorem 5.1. *Let U be a unicyclic (n, n_1)-graph. Then*

$$M_1(U) \geq 4n + (n + n_1) \left\lfloor \frac{n}{n - n_1} \right\rfloor - (n - n_1) \left\lfloor \frac{n}{n - n_1} \right\rfloor^2 . \tag{5.2}$$

Equality in (5.2) is attained if and only if U consists of n_1 pendent vertices, $n_t = (n - n_1) \left\lfloor \frac{n}{n-n_1} \right\rfloor - n_1$ vertices of degree $t = \left\lfloor \frac{n}{n-n_1} \right\rfloor + 1$, and $n_{t+1} = n - (n - n_1) \left\lfloor \frac{n}{n-n_1} \right\rfloor$ vertices of degree $t + 1$.

Unicyclic (n, n_1)-graphs with minimal first Zagreb index, of the form specified in Theorem 5.1, exist for any value of n and n_1, provided $n \geq 3$ and $n_1 \geq 0$.

Theorem 5.2. [14] *Let B be a bicyclic (n, n_1)-graph. Then*

$$M_1(B) \geq 4n + 6 + (n + n_1 + 4) \left\lfloor \frac{n+2}{n - n_1} \right\rfloor - (n - n_1) \left\lfloor \frac{n+2}{n - n_1} \right\rfloor^2 . \tag{5.3}$$

Equality in (5.3) is attained if and only if B consists of n_1 pendent vertices, $n_t = (n-n_1) \left\lfloor \frac{n+2}{n-n_1} \right\rfloor - n_1 - 2$ vertices of degree $t = \left\lfloor \frac{n+2}{n-n_1} \right\rfloor + 1$, and $n_{t+1} = n + 2 - (n - n_1) \left\lfloor \frac{n+2}{n-n_1} \right\rfloor$ vertices of degree $t + 1$.

Bicyclic (n, n_1)-graphs with minimal first Zagreb index, of the form specified in Theorem 5.2, exist for any value of n and n_1, provided $n \geq 4$ and $n_1 \geq 0$.

Also for any value of γ greater than 2, structural characterizations of γ-cyclic (n, n_1)-graphs with minimal first Zagreb index can be achieved in a fully analogous manner. However, when considering classes of graphs having a more complicated cyclic structure, one first has to check if condition (5.1) can be satisfied at all, which needs not always be the case.

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