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Bounding the First Zagreb Index of a Tree in Term of Its Repetition Number

Hong Lin[a,*], Jianguo Qian[b]

[a] *School of Sciences, Jimei University, Xiamen, Fujian, 361021, P.R.China*

[b] *School of Mathematics, Xiamen University, Xiamen, Fujian, 361005, P.R.China*

linhong@jmu.edu.cn, jgqian@xmu.edu.cn

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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. The repetition number of a graph is the maximum multiplicity in the list of its vertex degrees. In this note, we bound the first Zagreb index of a tree from both below and above by expressions depending solely on its repetition number.

1 Introduction

All graphs considered in this paper are simple and connected graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex v in G is the number of edges of G incident with v. The degree sequence of a graph is the non-increasing sequence of its vertex degrees. In a tree, a vertex of degree one is called a *pendent vertex*, and a vertex of degree at least three is called a *branching vertex*. As usual, S_n and P_n denote, respectively, the star and the path on n vertices. The first Zagreb index, defined as

*Corresponding author.

$$M_1(G) = \sum_{u \in V(G)} (d_G(u))^2,$$

is a widely studied degree-based topological index which was introduced by Gutman and Trinajstić [9] in 1972 and elaborated in [10]. It is an important molecular descriptor and has been closely correlated with many chemical properties. Chemists are often interested in the first Zagreb index of certain trees which represent some acyclic molecular structures. Gutman and Das summarized the main mathematical properties of M_1 in the survey [8]. For more results on this topic, we refer the readers the papers [2, 4–7, 12–14] and the recent survey [1].

Motivated by the well-known fact in graph theory which states that every graph (with no loops or multiedges) has two vertices with the same degree, Caro and West [3] defined *the repetition number* $rep(G)$ of a graph G to be the maximum multiplicity in the list of its vertex degrees. The main work of [3] is to established various lower bounds on $rep(G)$ for trees, maximal outerplanar graphs, planar triangulations, and claw-free graphs.

Roughly speaking, the repetition number provides a measure of regularity of a simple graph. For an $n-$vertex graph G, the largest possible value of $rep(G)$ is n. If $rep(G) = n$, then G is regular. It is interesting that both the first Zagreb index and the repetition number are degree-based invariants of graphs. The purpose of the present paper is to find some relationship between the two graph invariants, perhaps one possible research direction is to determine the upper bound and lower bound of the first Zagreb index of trees with given repetition number.

In [6,7], Goubko and Gutman established a remarkable result bounding the minimum value of M_1 of a tree in term of the number of pendent vertices, and only with this parameter. Another purpose of the present paper is provide a result with the fiavor of such type.

To state the results of this paper, we need some further terminologies and notations.

Let n be a positive integer. A sequence of positive integers $(n_1, n_2, ..., n_k)$ with $n_1 \geq n_2 \geq ... \geq n_k \geq 1$ is said to be a *partition* of n if $n = n_1 + n_2 + ... + n_k$. The set of all partitions of n is denoted by $\mathbb{P}_n$. For more details on this topic, we refer the readers to the Chapter 4 of [11]. For a positive integer n, we define a function $f(n)$ as follows:

$$f(n) = max\{(n_1 + 2)^2 + (n_2 + 2)^2 + ... + (n_k + 2)^2 \mid 1 \leq k \leq n, (n_1, n_2, ..., n_k) \in \mathbb{P}_n\}.$$

In the sequel, for convenience of discussion, for a tree T we always use the symbol $\Delta(T)$ to denote the maximum degree of T, and use the symbol $r_i(T)$ to denote the number of vertices of T with degree i, where $1 \leq i \leq \Delta(T)$.

Let $\mathbb{T}_r$ be the set of trees with repetition number r. Now we can state the main result of the present paper.

Theorem 1.1. Let $T \in \mathbb{T}_r$, where $r \geq 4$. Then

$$4r + 2 \leq M_1(T) \leq f(r - 2) + 5r.$$

The lower bound is achieved if and only if $T = P_{r+2}$, and if T^* is a tree satisfying the upper bound, then $r_1(T^*) = r_2(T^*) = rep(T^*)$.

The rest of this paper is organized as follows. In Section 2, we provide some useful results which will help to prove our main result. We close this paper in Section 3 by proving Theorem 1.1 and proposing some new problems for research.

2 Preliminaries

The following theorem obtained by Gutman and Das [8] is an elementary result on the first Zagreb index of trees.

Theorem 2.1. Let T be a tree on n vertices, then

$$4n - 6 \leq M_1(T) \leq n(n - 1).$$

The lower bound is attained if and only if $T = P_n$ and the upper bound is attained if and only if $T = S_n$.

A tree is called a *caterpillar* if the removal of all pendent vertices results in a path. In [12], one author of the present paper obtained the following result (see Lemma 3 of [12]).

Lemma 2.2 ([12]). Suppose T is an $n-$vertex non-caterpillar, then there exists an $n-$vertex caterpillar T' such that T' and T have the same degree sequence.

Lemma 2.3. For any tree T , $rep(T) = max\{r_1(T), r_2(T)\}$.

Proof. Suppose, to the contrary, that $rep(T) = r_i(T)$ holds for some $3 \leq i \leq \Delta(T)$. Set $\Delta(T) = \Delta$ and $r_t = r_t(T)$ for each $1 \leq t \leq \Delta(T)$. Assume that T has n vertices (and thus with $n-1$ edges), then

$$r_1 + r_2 + ... + r_\Delta = n. \tag{1}$$

By the handshaking lemma,

$$r_1 + 2r_2 + ... + \Delta r_\Delta = 2 \mid E(T) \mid = 2(n-1). \tag{2}$$

Now,

$2(n-1)$

$= r_1 + 2r_2 + 3r_3 + ... + \Delta r_\Delta \quad$ (by (2))

$= (2r_1 + 2r_2 + 3r_3 + ... + (i-1)r_{i-1} + (i-1)r_i + (i+1)r_{i+1} + ... + \Delta r_\Delta) + (r_i - r_1)$

$\geq 2(r_1 + r_2 + r_3 + ... + r_{i-1} + r_i + r_{i+1} + ... + r_\Delta) + (r_i - r_1)$ (since $i \geq 3$)

$= 2n + (r_i - r_1)$ (by (1))

$\geq 2n$, (since $r_i = rep(T) \geq r_1$)

a contradiction. □

3 Proof of Theorem 1.1 and further discussion

Proof. Set $\mid V(T) \mid= n$. Since $T \in \mathbb{T}_r$, $r \geq 4$, thus $n \geq r+1 \geq 5$. If $n = r+1$, by Lemma 2.3, T has exactly $(n-1) = r$ vertices with the same degree one or two. Notice that T has at least two pendent vertices, it is easy to see that $T = S_{r+1}$.

If $n \geq r+2$, note that $P_{r+2} \in \mathbb{T}_r$, by Theorem 2.1,

$$M_1(T) \geq M_1(P_n) \geq M_1(P_{r+2}) = 4(r+2) - 6 = 4r + 2,$$

with equality if and only if $n = r + 2$ and $T = P_{r+2}$.

Therefore, the tree with the minimal first Zagreb index in $\mathbb{T}_r$ is either S_{r+1} or P_{r+2}. Notice that

$M_1(S_{r+1}) - M_1(P_{r+2})$

$=(r^2 + r) - (4r + 2) = r(r - 3) - 2 > 0.\quad$ (since $r \geq 4$)

So P_{r+2} is the sole graph in $\mathbb{T}_r$ that attains the minimal value of the first Zagreb index.

Now we turn to determine the upper bound of $M_1(T)$.

Let T^* be a tree with the maximal first Zagreb index in $\mathbb{T}_r$ and let π be its degree sequence. By Lemma 2.2, we can always find a caterpillar $T_c^* \in \mathbb{T}_r$ with π as its degree sequence (if T^* is a caterpillar, we may set $T_c^* = T^*$). Consequently,

$$M_1(T^*) = M_1(T_c^*).$$

Set $r_i = r_i(T_c^*)$ for each $i \leq \Delta(T_c^*)$.

Claim 1. T_c^* has at least one branching vertex.

Suppose, to the contrary, T_c^* contains no branching vertex. Then T_c^* is a path. Since $rep(T_c^*) = r$, thus $T_c^* = P_{r+2}$. Note that $S_{r+1} \in \mathbb{T}_r$, but

$M_1(S_{r+1}) - M_1(P_{r+2}) = (r^2 + r) - (4r + 2) = r(r - 3) - 2 > 0,$ (since $r \geq 4$)

contradicting to the maximality of T_c^*.

Claim 2. $r_1 \geq r_2$.

Suppose, to the contrary, $r_1 < r_2$. Let T_1 be the tree obtained from T_c^* by adding a new vertex x and joining x to one branching vertex u of T_c^*. By Lemma 2.3, it is clear that $T_1 \in \mathbb{T}_r$, but

$M_1(T_1) - M_1(T_c^*) = d_{T_1}^2(u) - d_{T_c^*}^2(u) + d_{T_1}^2(x) = [d_{T_c^*}(u) + 1]^2 - d_{T_c^*}^2(u) + 1 = 2d_{T_c^*}(u) + 2 > 0,$

contradicting to the maximality of T_c^*.

Claim 3. $r_2 \geq r_1$.

Suppose, to the contrary, $r_2 < r_1$. Let v be a pendent vertex of T_c^* and u the unique neighbor of v. Let T_2 be the tree obtained from T_c^* by inserting a new vertex y on the edge uv. By Lemma 2.3, it is clear that $T_2 \in \mathbb{T}_r$, but

$M_1(T_2) - M_1(T_c^*) = d_{T_2}^2(y) = 4,$

contradicting to the maximality of T_c^*.

Now from Claim 2, Claim 3 and Lemma 2.3, we arrive at

$$r_1 = r_2 = rep(T_c^*) = rep(T^*) = r. \tag{3}$$

Let $P = y_0 y_1 y_2 ... y_{l-1} y_l$ be a longest path of T_c^*, then y_0, y_l are two pendent vertices. Recall that T_c^* is a caterpillar, thus each vertex of degree two lies on P. Now by (3), we can deduce that for the remaining $r-2$ pendent vertices (other than y_0 and y_l), each is adjacent to some y_i for some $1 \leq i \leq l-1$.

Assume that T_c^* has k branching vertices, by Claim 1 and (3), $k \geq 1$ and T_c^* has exactly $k+2r$ vertices. We may further assume that $(d_1, d_2, ..., d_{k+2r})$ is the degree sequence of T_c^* with

$$d_1 \geq d_2 \geq ... \geq d_k \geq 3 > d_{k+1} = ... = d_{k+r} = 2 > d_{k+r+1} = ... = d_{k+2r} = 1.$$

Note that each branching vertex of T_c^* has exactly two neighbors in the path $P = y_0 y_1 y_2 ... y_{l-1} y_l$ and each pendent vertex (other than y_0 and y_l) is adjacent to one branching vertex of T_c^*, thus

$$(d_1 - 2) + (d_2 - 2) + ...(d_k - 2) = r - 2, \tag{4}$$

namely, $(d_1 - 2, d_2 - 2, ..., d_k - 2)$ is a partition of $r-2$.
This leads to

$M_1(T_c^*)$
$= d_1^2 + d_2^2 + ...d_k^2 + 4r + r$
$= d_1^2 + d_2^2 + ...d_k^2 + 5r$
$= f(r-2) + 5r$, (by the maximality of T_c^* and the definition of the function $f(n)$)
by which the proof of Theorem 1.1 is completed. $\square$

It is somewhat mysterious that we know much less about the structural properties for the extremal trees with the maximum value of M_1 of trees in the class $\mathbb{T}_r$ other than that $r_1(T) = r_2(T) = rep(T)$ for each extremal tree T. To get more information about the extremal trees, we need some further notation.

Let π be a partition of a positive integer n, we use the symbol $p(\pi, n)$ to denote the number of parts of the partition π. For examples, $\pi_1 = (3, 1, 1, 1)$ is a partition of 6 with 4 parts, so $p(\pi_1, 6) = 4$ and $\pi_2 = (3, 3, 1)$ is a partition of 7 with 3 parts and hence $p(\pi_2, 7) = 3$. Clearly, for any positive integer n, two specific partitions (n) and $(\underbrace{1, 1, ..., 1}_{n})$ are two partitions of n with the minimal and maximal values of $p(\pi, n)$ respectively. So for a partition $\pi \in \mathbb{P}_n$, we have

$$1 \leq p(\pi, n) \leq n. \tag{5}$$

Corollary 3.1. Let $T^* \in \mathbb{T}_r$ $(r \geq 4)$ be a tree satisfying the right-hand side equality in Theorem 1.1, namely, $M_1(T^*) = f(r-2) + 5r$, then

$$2r + 1 \leq| V(T^*) |\leq 3r - 2. \tag{6}$$

Proof. From the proof of Theorem 1.1, we know that the degree sequence of T^* has the following form

$$(\underbrace{d_1, d_2, ..., d_k}_{k}, \underbrace{2, ..., 2}_{r}, \underbrace{1, ..., 1}_{r}),$$

where k is the number of branching vertices of T^* and $(d_1-2, d_2-2, ..., d_k-2)$ is a partition of $r-2$ such that $d_1^2+d_1^2+...+d_k^2 = f(r-2)$. So according to (5),

$$1 \leq k \leq r - 2.$$

Note that $| V(T^*) |= k + 2r$, hence $2r + 1 \leq| V(T^*) |\leq 3r - 2$. $\square$

Remark. We remark that for some specific integer r, the extremal trees in $\mathbb{T}_r$ realizing the upper bound in Theorem 1 might have different number of vertices. In case of $r = 6$, the set of all partitions of 4 is $\mathbb{P}_4 = \{(4), (3, 1), (2, 2), (2, 1, 1), (1, 1, 1, 1)\}$. It is easily checked that $f(r-2) = f(4) = 36$ is attained by two partitions (4) and (1, 1, 1, 1). In the class $\mathbb{T}_6$, the maximum value of M_1 is $f(r-4) + 5r = f(4) + 30 = 66$. In Figure 1, two trees in $\mathbb{T}_6$ with maximum value of M_1 are depicted. The tree T_1 has $2r + 1 = 13$ (attains the lower bound in (6)) vertices and the degree sequence (6, 2, 2, 2, 2, 2, 2, 1, 1, 1, 1, 1, 1), while the tree T_2 possesses $3r - 2 = 16$ vertices (attains the upper bound in (6)) and the degree sequence (3, 3, 3, 3, 2, 2, 2, 2, 2, 2, 1, 1, 1, 1, 1, 1).

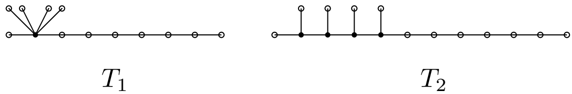

Figure 1. Two trees T_1 and T_2 in $\mathbb{T}_6$ with maximum value of $M_1 = 66$.

In the end of the paper, we leave the following problems which might be worthwhile to study.

Problem. Could such type results as stated in Theorem 1.1 be extended to some classes of graphs with more cycles, such as unicyclic and bicyclic graphs?

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