MAXIMAL GRAPHS OF THE FIRST REVERSE ZAGREB BETA INDEX

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ABSTRACT. The reverse vertex degree of a vertex v of a simple connected graph G defined as; $c_v = \Delta - d_v + 1$ where Δ denotes the largest of all degrees of vertices of G and d_v denotes the number of edges incident to v. The first reverse Zagreb beta index of a simple connected graph G defined as; $CM_1^\beta(G) = \sum_{uv \in E(G)} (c_u + c_v)$. In this paper we

characterized maximal graphs with respect to the first reverse Zagreb beta index.

Keywords: Reverse vertex degree, Reverse Zagreb indices, First reverse Zagreb beta index.

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1. INTRODUCTION

A topological index ,which is a graph invariant it does not depend on the labeling or pictorial representation of the graph, is a numerical parameter mathematically derived from the graph structure. The topological indices of molecular graphs are widely used for establishing correlations between the structure of a molecular compound and its physicochemical properties or biological activity. These indices are used in quantitive structure property relations (QSPR) research. The first distance based topological index was proposed by Wiener in 1947 for modeling physical properties of alcanes [1], and after him, hundred topological indices were defined by chemists and mathematicians and so many properties of chemical structures were studied. More than forty years ago Gutman and Trinajstić defined Zagreb indices which are degree based topological indices [2]. These topological indices were proposed to be measures of branching of the carbon-atom skeleton in [3]. The first and second Zagreb indices of a simple connected graph G defined as follows;

$$M_1\left(G\right) = \sum_{u \in V(G)} d_u^2$$

and

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v$$

where u, V(G), uv and E(G) denotes a vertex of G, the vertex set of G, an edge of G and the edge set of G, respectively. For details of the chemical applications and the

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mathematical theory of the Zagreb indices, see the surveys [4, 5, 6, 7]. For the another version of the first Zagreb index;

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$$

see in [7].

Recently, reverse vertex degree of a vertex and reverse Zagreb indices of a simple connected graph have been defined in [8]. The reverse vertex degree of a vertex v of a simple connected graph G defined as;

$$c_v = \Delta - d_v + 1$$

where Δ denotes the largest of all degrees of vertices of G and d_v denotes the number of edges incident to v. The total reverse vertex degree defined as;

$$TR\left(G\right) = \sum_{u \in V(G)} c_u$$

The first reverse Zagreb alpha index of a simple connected graph G defined as;

$$CM_1^{\alpha}\left(G\right) = \sum_{u \in V(G)} c_u^2$$

The first reverse Zagreb beta index of a simple connected graph G defined as;

$$CM_1^\beta(G) = \sum_{uv \in E(G)} (c_u + c_v)$$

And the second reverse Zagreb index of a simple connected graph G defined as;

$$CM_2(G) = \sum_{uv \in E(G)} c_u c_u$$

Maximum chemical trees of the second Zagreb index were characterized in [8]. The reverse Zagreb indices of Cartesian product of two graphs were computed in [9]. The aim of this paper is to characterize maximal graphs with respect to the first reverse Zagreb beta index.

2. Maximal graphs with respect to the first reverse Zagreb beta index

In this section our goal is to characterize maximal graphs of the first reverse Zagreb beta index.

Theorem 2.1. Let $n \ge 4$ be an even integer and $G \cong G_{n/2}$ be n-vertex n/2-regular graph. Then, $L \cong G + v$ ($v \notin V(G)$) has the maximal CM_1^β -value among the all n + 1-vertex simple connected graphs.

Proof. If we show that adding any edge to L or taking any edge from L decreasing the first reverse Zagreb beta index value then we prove the claim. For this, we consider two cases.

Case 1: Let u, s be non adjacent vertices of L. Let S be a graph obtained by making adjacent u to s, e = us. Clearly c_u and c_s values decreasing by one since the degrees of uand s increasing by one in S. That is, from the definition of the reverse vertex degree for the graph S, we get that $c_u = c_v = n - (n/2 + 2) + 1 = n/2 - 1$ and for the edge e = us, $c_u + c_v = n - 2$. Therefore CM_1^β -value of L decreased by n + 2 and increased by n + 2 since every vertex of L except from v has n/2 + 1 neighbors. Hence $CM_1^\beta(L) - CM_1^\beta(S) = 4 > 0$. Case 2: Let e = us be an edge of L and $S \cong G - e$. In this case there are two subcases. Subcase 1: Let u = v. Then Δ reduced by one. Therefore reverse degrees of all vertices of S decreased by one. Hence the first reverse Zagreb beta value of L is greater than the first reverse Zagreb beta value of S.

Subcase 2: Let $u \neq v$ and $s \neq v$. Then the reverse degree of the vertices u and s decreasing by one. Thus the first reverse Zagreb beta index value of the graph L is greater than the first reverse Zagreb beta index value of the graph S.

Corollary 2.1. Let L be n + 1 vertex graph which is specified in Theorem 2.1. Then, $CM_1^{\beta}(L) = \frac{1}{4}n(n^2 + 6n + 4).$

Proof. There are two kind of edges in L. The vertices of the first kind of edges have degree n/2 + 1 and have reverse degree n/2. The vertices of the second kind of edges have degree n/2 + 1, n and have reverse degree n/2 and 1. Clearly, the number of the first kind of edges are $n^2/4$ and the number of the second kind of edges are n. From this,

$$CM_1^{\beta}(L) = \frac{n^2}{4}(n/2 + n/2) + n((n/2 + 1) + n)$$
$$= \frac{n^3}{4} + \frac{n}{2}(3n + 2) = \frac{n}{4}(n^2 + 6n + 4)$$

can be written by using the definition of the first reverse Zagreb beta index.

Theorem 2.2. Let $n \ge 5$ be an odd integer and G be n-vertex connected graph in which all the vertices have the degree $\lfloor \frac{n}{2} \rfloor$ except from the one vertex say s which has the degree $\lfloor \frac{n}{2} \rfloor - 1$. Then, the graph $L \cong G + v$ ($v \notin V(G)$) has the maximal CM_1^β value.

Proof. Let n = 2r + 1, therefore $\lfloor \frac{n}{2} \rfloor = r$. If we show that adding any edge to L or taking any edge from L decreases the first reverse Zagreb beta index value then we prove the claim as in the proof of Theorem 2.1. There are two cases.

Case 1: Let $S \cong L + e$. There are two possibilities of the choice of e.

Subcase 1: Let u be a vertex which of $d_u = \lfloor \frac{n}{2} \rfloor + 1 = r + 1$, s be the vertex which of $d_s = \lfloor \frac{n}{2} \rfloor = r$ in V(L) and e = us. Therefore the reverse vertex degrees of the vertices u and s decreased by one. Hence the value of the first reverse Zagreb beta index value of the graph S decreased by 2r + 1 since the sum of the number of the neighbors of the vertices of u and s is 2r + 1 in L and increased by 2r - 1 since $c_u + c - v = 2r + 1$ with respect to the first reverse Zagreb alpha index value of L. Thus, $CM_1^{\beta}(L) - CM_1^{\beta}(S) = 2 > 0$.

Subcase 2: Let u_1 and u_2 be the vertices which of $d_{u_1} = d_{u_2} = \lfloor \frac{n}{2} \rfloor + 1 = r + 1$ in V(L) and $e = u_1 u_2$. Therefore the reverse vertex degrees of the vertices u_1 and u_2 decreased by one. Hence the value of the first reverse Zagreb beta index value of the graph S decreased by 2r + 2 since the sum of the number of the neighbors of the vertices of u_1 and u_2 is 2r + 2 in L and increased by 2r since $c_{u_1} + c_{u_2} = 2r$ with respect to the first reverse Zagreb beta index value of L. Thus, $CM_1^{\beta}(L) - CM_1^{\beta}(S) = 2 > 0$.

Case 2: Let $S \cong L - e$ and $u \in V(L)$ which of $d_u = \lfloor \frac{n}{2} \rfloor + 1$. In this case there are only four possibilities of the choice of e.

Subcase 1 : Let e = uv. Then Δ reduced by one. Therefore reverse degrees of all vertices of S decreasing by one. Hence the first reverse Zagreb beta index value of L is greater than the first reverse Zagreb beta index value of S.

Subcase 2 : Let e = sv. Then Δ reduced by one. Therefore reverse degrees of all vertices of S decreasing by one. Hence the first reverse Zagreb beta index value of L is greater than the first reverse Zagreb beta index value of S.

Subcase 3 : Let e = us. Then the reverse degree of the vertices u and s decreasing by one. Hence the first reverse Zagreb beta index value of L is greater than the first reverse Zagreb beta index value of S.

Subcase 4 : Let $e = u_1 u_2$. Then the reverse degree of the vertices u_1 and u_2 decreased by one. Hence the first reverse Zagreb beta index value of L is greater than the first reverse Zagreb beta index value of S.

Corollary 2.2. Let L be n + 1-vertex graph which specified in Theorem 2.2. Then, $CM_1^{\beta}(L) = \frac{1}{4}(n^3 + 2n^2 + n - 8).$

Proof. Let n = 2r + 1. There are four kind of edges in L. The vertices of the first kind of edges have degree $\lfloor \frac{n}{2} \rfloor + 1 = r + 1$ and and the reverse degree of these vertices are r + 1. The vertices of the second kind of edges have degrees $\lfloor \frac{n}{2} \rfloor + 1 = r + 1$ and $\lfloor \frac{n}{2} \rfloor = r$. And the reverse degree of these vertices are r + 1 and r + 2, respectively. The vertices of the third kind of edges have degrees $\lfloor \frac{n}{2} \rfloor + 1 = r + 1$ and 1, respectively. The vertices of the fourth kind of edge have degrees $\lfloor \frac{n}{2} \rfloor + 1 = r + 1$ and 2r + 1 and the reverse degree of these vertices are r + 1 and 1, respectively. The vertices of the fourth kind of edge have degrees $\lfloor \frac{n}{2} \rfloor = r$ and 2r + 1 and the reverse degree of these vertices are r + 2 and 1, respectively. Clearly, the number of the first kind of edges are $\frac{1}{2}(2r+1)(r-1)$, the number of the second kind of edges are r - 1, the number of the third kind of edges 2r and the number of the fourth kind of edge is 1. From these facts we get that,

$$CM_1^{\beta}(L) = \frac{1}{2}(2r+1)(r-1)((r+1) + (r+1))$$

+(r-1)((r+1) + (r+2)) + 2r((r+1) + 1) + ((r+2) + 1)
= (2r+1)(r-1)(r+1) + (r-1)(2r+3) + 2r(r+2) + r + 3
= (2r+1)(r^2 - 1) + 2r^2 + r - 3 + 2r^2 + 5r + 3
= 2r^3 + r^2 - 2r - 1 + 4r^2 + 6r = 2r^3 + 5r^2 + 4r - 1
= 2\frac{(n-1)^3}{8} + 5\frac{(n-1)^2}{4} + 4\frac{n-1}{2} - 1
= \frac{1}{4}((n-1)^3 + 5(n-1)^2 + 8(n-1) - 4)
= \frac{1}{4}(n^3 + 2n^2 + n - 8)

3. CONCLUSION

In this paper we found two classes of graph which are maximal with respect to the first reverse Zagreb beta index. It would be interesting to find that the graphs which are maximum with respect to the first reverse Zagreb beta index. It would also be interesting to find that the graphs which are maximum with respect to the second reverse Zagreb index for further studies.

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