Consolidated Extremal Combinatorics Results among the Class of Degree-Based Graphs to Zagreb Indices with the Given Diameter

Section A-Research paper



Consolidated Extremal Combinatorics Results among the Class of Degree-Based Graphs to Zagreb Indices with the Given Diameter

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Abstract

In this paper, we discussed all extremal connected graphs among the class of bicyclic and tricyclic graph by using the first general Zagreb index $R^0_{\alpha}(G)$ for $0 > \alpha > 1$ minimum and maximum for $0 < \alpha < 1$, also for first multiplicative Zagreb index $\Pi_{u \in v(G)}(d(u))^{\alpha}$ for minimum $\alpha < 0$ and maximum for $\alpha > 0$, maximum second Zagreb multiplicative index $\Pi_2(G)$ and minimum first coindex $M_1(G)$ among above mentioned graphs with the given diameter respectively.

Keywords Extremal graphs, bicyclic, tricyclic, Zagreb index, multiplicative Zagreb.

Subject Classification Codes 05C35, 05C40, 05C62, 05C90, 46A63.

1. Introduction

In this paper, all the graphs are finite, connected and undirected graphs. Let G = (V, E) be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \dots, e_n\}$ where |V(G)| = n and |E(G)| = m. Two vertices of G, connected by an edge, are said to be "adjacent". If m = n + c - 1 for c = 2, 3, 4 is called bicycle and tricyclic and tetracyclic graphs respectively. The $d_G(v)$ or d(v) is short form of the degree of a vertex in G. Let $d(v_i) = d_i$ be the degree of the vertex v_i for $i = 1, 2, 3, \dots, n$. Suppose $(d(v_1) \ge d(v_2) \ge d(v_3) \dots \ge d(v_n)$. A non-negative integer $\prod = (d_1, d_2, \dots, d_n)$ is called graphical sequence of G (\prod is also called degree sequence of G). A vertex having degree one is called pendant vertex. While a vertex with $deg \ge 2$ is called a non-pendant vertex. Let G = (V, E) be the c-cyclic graph if |E| = |v| + c - 1, where c is a non-negative integer. In this case $N_G(V)$ is the neighborhood set of V and sometime denoted as $|N_G(V)| = d_G(v) = d(v)$ where $N_G(V) = \{u: uv \in E(G)\}$ for $u, v \in V(G)$ where d(u, v) denotes the distance between vertices u and v. Distance here mean is the number of edges in a shortest path from u to v. The number of pendant vertices is denoted by P(G). The reduced graph obtained from G denoted by R(G) while N_H be the set of non pendant vertices of H in G.

In 1972, Gutman and Trinajstic [1] interject the first Zagreb index $M_1(G)$ of a graph G represented the sum of the squares of the degrees of all vertices of G.

$$M_1(G) = \sum_{i=1}^n d_i^2$$
 (1)

It is mostly studied topological index [2]. They also used these results for total \prod electron energy by using symbole du instead of δu for the degree of the vertex u. Also M_1 also known as first Zagreb group index [3] and some authors call M_1 the Gutman index [4].

Doslic [5] defined the first Zagreb coindex $M_1(G)$ for degrees of vertices u and v such that

$$\underline{M_1(G)} = \sum_{uv \notin E(G)} \left(d(u) + d(v) \right)$$
⁽²⁾

Li and Zheng [6] defined the first general Zagreb Index R_{α} (G) find generalization forms such as

$$R^0_{\alpha}(G) = \sum_{u \in \mathcal{V}(G)} (du)^{\alpha} \tag{3}$$

Where α denotes a real number as α parameter. In particular case [7] Inverse degree of general form the present as

$$R^0_{-1}(G) = \sum_{u \in \nu(G)} (du)^{-1} = \sum_{u \in \nu(G)} (\frac{1}{du})$$
(4)

With the concern to this, some statements are required because results obtained in the theory of Zagreb indices are compiled in the reviews. According to chemical point of view of M_1 and M_2 are outlined in the survey. According to the information about inspection by pointing out the mathematical connections of M_1 and M_2 are the same. So, the second Zagreb index $M_2(G)$ are also defined as fellows by Bolian and Ivan Gutman [8]

$$M_2(G) = \sum_{vi,vj \in E(G)} d_i d_j \tag{5}$$

The second modified Zagreb index $M_2^*(G)$ is equal to the sum of the reciprocal products of degrees adjacent to pair vertices [9] and denoted by formula.

$$M_2^*(G) = \sum_{vi,vj \in E(G)} \frac{1}{d_i d_j}$$
(6)

Narumi and Katayama considered the product of vertices degrees as

$$K(G) = \pi_{\nu} d_{\nu}(G) \tag{7}$$

In 2010, the following results obtained by Todeschini and Consonni [10] about the first multiplicative Zagreb index Π_1 (*G*) and second multiplicative Zagreb index Π_2 (*G*) of the graph G such that

$$\Pi_1 (G) = \Pi_{u \in v(G)} d^2(u) \tag{8}$$

$$\Pi_2 (G) = \Pi_{u-v} \ d_u(G).d_v(G) \tag{9}$$

$$\Pi_2 (G) = \Pi_{u \in \mathcal{V}(G)} (du)^{du} \tag{10}$$

Modified Zagreb multiplied index represented by $\Pi_1^*(G)$

$$\Pi_1^*(G) = \Pi_{u-\nu}[d_u(G) + d_\nu(G)]$$
(11)

 $\Pi_1^*(G)$ very recently the general multiplicative Zagreb Index $\Pi^{\alpha}(G)$ was defined as [11]

$$I^{\alpha}(G) = \Pi_{u \in v(G)}(d(u))^{\alpha}$$
(12)

Obviously, the Narumi Katayama index and the first multiplicative Zagreb index are simply related as

$$\Pi_1 (G) = NK (G)^2 \tag{13}$$

It has observed that some quantities often referred to as general Zagreb index [11], for $\alpha = 2$ the first Zagreb index [12, 13] usually represented as $\sum_{u} (d_u)^2$.

Later Erodos and Bollobas (generalized) introduced the generalized form for any real number α .

$$R_{\alpha}(G) = \sum_{uv \in E(G)} (d_u d_v)^{\alpha}$$
(14)

If we take $\alpha = 1$ in the equation [14] the R_{α} (G) is also called the second Zagreb index. If we take $\alpha = 3$ in the equation (3) then we can write it as

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$$R^0_\alpha(G) = \sum_{u \in v(G)} (du)^3 \tag{15}$$

Then equation (15) is also called the forgotten topological index or shortly the F-Index [15]. Many researchers are charmed by the concept of finding extremal results of vertex degree based undirected graphs to various Zagreb indices having the maximum and minimum values of the corresponding indices [16]. At the present time there are a lot of articles related to Zagreb indices in different areas between Chemistry and Mathematics [17-19].

As usually for a graph G is the first Zagreb index M_1 and second Zagreb index M_2 are defined as:

$$M_1 = M_1 (G) = \sum_{u \in v(G)} d(v)^2$$
(16)

$$M_2 = M_2 (G) = \sum_{uv \in E(G)} d(u) d(v)$$
(17)

Where d(u) denotes the degree of the vertex u of G and d(v) represent the degree of the vertex v of G.

2. Material and Methods

It is a universal issue to compare the values of the Zagreb indices on the same graph. The first Zagreb index M_1 have order $O(n^3)(n = O(n)$ and the second Zagreb index M_2 have order $O(n^4) O(n^2) = m$ edge. It means we can compare M_1 /n with M_2 /m instead of M_1 and M_2 . The Auto Graphic system [20] the theorized M_1 /n $\leq M_2$ /m, where n = |V(G)| and m = |(E(G))| for simple connected undirected graphs. Hansen and vukicevic [21] showed, it is true for chemical graphs and it is not true for general graphs. In this paper, we construct counter examples of connected bicyclic and tricyclic graphs. If we discuss the finite, undirected graph such that $xy \in E(G)$, then we can say y is the neighborhood of x and represented by $N_G(x)$ which is the set of neighborhoods set of x and is also denoted by $N_G[x] = N_G(x)U\{x\}$ also $d_G(x) = |N_G(x)|$ and is called the degree of x. If n_i the number of vertices of degree i in G then the number of edges represented by m_{ij} who connect vertices of degree i and j.

3. Results and Discussion

3.1. Connected bicycle graphs having no pendant vertices with comparable Zagreb indices.

We discuss the following theorems for better understanding.

Theorem 3.1.1: Let M_1 and M_2 be two first and second Zagreb indices having order $O(n^3) = O(n) = n$ vertices and $O(n^4) = O(n^2) = m$ edges simultaneously such that M_1 (G) $/n \le M_2$ (G)/m is true for any chemical graph [20]. The bound is tight for a simple connected bicyclic graph G with equality holds if and only if $G = K_{2,3}$.

Proof: According to the Figure 1-3, this theorem has three cases.



Figure 1



Figure 3

Case-1: In Figure 1, we have

 $n_2 = n - 1, n_4 = 1 m_{22} = n + 1 - 4 = n - 3$ and $m_{24} = 4$,

Then,

$$M_1(G) = 4n - 4 + 16 = 4n + 12 = 4(n + 3).$$

 $M_2(G) = 4 + 8(4) = 4n - 12 + 12 = 4n + 20.$

Since $n \ge 5$ we have $\frac{M_1(G)}{n} < \frac{M_2(G)}{m}$. Case-2: In Figure 2, we have

 $m_{33} = 1, m_{22} = m - 4$ and $m_{23} = 4$,

Then,

$$M_2(G) = 4m_{22} + 6m_{23} + 3^2 = 4(n-4) + 6(4) + 9 = 4(n-4) + 24 + 9 = 4n - 16 + 24 + 9,$$

 $M_2(G) = 4n + 17.$

Also, $n_2 = n - 2 \& n_3 = 2$ then we have

$$M_1(G) = 4n_2 + 9n_3 = 4(n-2) + 9(2) = 4n - 8 + 18 = 4n + 10.$$

Sub Case 2

If $m_{33} = 0$, $m_{22} = n + 1 - 6 = n - 5$, $m_{23} = 6$ and $M_2(G) = 4(n - 5) + 36 = 4n + 16$. For $n \ge 6$ we have $\frac{M_1(G)}{n} < \frac{M_2(G)}{m}$.

Case-3: In Figure 3, we have

$$n_3n_3 = 2$$
, $n_2 = n - 2$ then for
 $M_1(G) = 4n_2 + 9n_3 = 4(n - 2) + 9(2) = 4n - 8 + 18 = 4n + 10.$

Subcase if $m_{22} = n - 4$, $m_{23} = 4$, $m_{33} = 1$ then for

$$M_2(G) = 4m_{22} + 6m_{23} + 3^2 = 4(n-4) + 6(4) + 9 = 4n - 16 + 24 + 9.$$

$$M_2(G) = 4n - 16 + 33 = 4n + 17.$$

 $M_2(G) = 4n - 16 + 33 = 4n + 17.$ If $m_{33} = 0$ and $m_{22} = n + 1 - 6 = n - 5, m_{23} = 6$ then $M_2(G) = 4(n - 5) + 36 = 4n + 16.$ Since $n \ge 4$ we have $\frac{M_1(G)}{n} < \frac{M_2(G)}{m}$ for if $m_{33} = 1$ also for $n \ge 5$ we have $\frac{M_1(G)}{n} \le \frac{M_2(G)}{m}$ with the equality holds if and only if n = 5 i.e $G = K_{2,3}$ as required.

3.2. Comparing results of Zagreb indices of connected bicyclic graph.

Theorem 3.2.1: Let G be a connected bicyclic graph having pendant vertices. For any pendant vertex $V \in H(G)$ such that $N_G(v) = \{u_1, u_2, \dots, u_k\}$ for $k \ge 2$ where $A = \{G: d_G(u_1) = 2, d_G(u_i) = 1 \text{ for } i = 2, 3 \dots k\}$.

Lamma 3.2.2: If A= {G: $d(u_1)=2$, $d_G(u_1)=1$ for $i = 2, 3 \dots k$ } then G \notin A is a connected bicyclic graph with pendent vertices having a subgraph F such that G - F \notin A where G-F is a connected bicyclic graph. *Proof:* Let us considered a vertex V ϵ H(G) such that V has at least two pendant vertices. let u be the adjacent pendant vertex of v. Then G-U \notin A where G - U is a connected bicyclic graph.



Here w is a pendant vertex such that G - W \notin A, Let F=W then G - F \notin A becauseG-F is a connected bicyclic graph. Let H(G) has a vertex which is adjacent to a particular pendant vertex.

For each pendant vertex x such that G - x ϵ A from Figure 4 d(v_i)=2, i=0,2,3....t d(v_1)=3, d($v_{t=1}$)≥3 or t≥2 and d(u_i)=1 and j=0,1.

Let $N(v_{t+1}) = \{v_t, w_1, w_2, \dots, w_s\}$ for $s \ge 2$, we have $d(w_i) \ge 2$, $i = 1, 2, 3, \dots, s$ for $d(w_1) = 1$, where w_1 is unique pendant vertex that is adjacent to v_{t+1} . Also, $G-w_1 \notin A$ for $s \ge 3$ is a contradiction. Now G is a connected bicyclic graph for s = 2. So, it is a clear v_{t+1} is not pendant vertex while all w_s are pendant vertices of the v_{t+1} . Therefore $G-w_1 \notin A$ a contradiction. From Figure 4 we can say

 $F = [\{u_0, u_1, v_0, v_1, v_2, \dots, v_{t+1}\} t \ge 2]$. If G - F \notin A then G - F is connected to a bicycle graph as required.

Corollary 3.2.3: The counter examples of connected bicyclic graphs 1-3 are given bellow. Example of bicycle with n=5 Vertices having diameter d=3 and find first and second Zagreb indices







Solution: $dv_5 = 1, dv_5 = 3, dv_4 = 4, dv_2 = dv_3 = 2.$ So, $\Pi(G) = (4,3,2,2,1)$ is graphical. First Zagreb index $M_1(G) = \text{sum of the sequence of all vertices in the graphs}$ $M_1(G) = d^2v_1 + d^2v_2 + d^2v_3 + d^2v_4 + d^2v_5$ $M_1(G) = 3^2 + 2^2 + 2^2 + 4^2 + 1^2 = 9 + 4 + 4 + 16 + 1 = 34.$

Second Zagreb index

$$\begin{split} M_2(g) &= \text{sum of the product of degrees of pair adjacent vertices in molecular graphs.} \\ M_2(g) &= (dv_1 * dv_2) + (dv_1 * dv_3) + (dv_1 * dv_4) + (dv_2 * dv_4) + (dv_3 * dv_4) + (dv_4 * dv_5) \\ M_2(g) &= (3*2) + (3*2) + (3*4) + (2*4) + (2*4) + (4*1) = 6 + 6 + 12 + 8 + 8 + 4 = 44. \end{split}$$

Second multiplicative z-index by Todeschini and Canzoni

 $\pi_2(G) = \pi_{u \in v(G)}(du)^{du} = (44)^{44}.$

Theorem 3.2.4: If G is an associated bicycle graph such that $G \notin A$ having n vertices an and edges m then $M_1(G) = M_2(G)$

$$\frac{M_1(G)}{n} \le \frac{M_2(G)}{m}$$

with the uniformity holds if and only if $G=K_{2,3}$ where $A= \{G: d_G(v_1)=2, d_G(v_i)=1 \text{ for } i=2,3...k\}$. <u>Proof</u>: Let G be connected bicyclic graph having no pendant vertices, by theorem 2.2.3 if and only if $G = K_{2,3}$ equality holds we have $\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m}$. Now we consider G as a connected bicyclic graph. We have m=n+1 then we prove it by mathematical induction on n.



$$d(v_1) = 2, d(v_2) = d(v_3) = d(v_4) = 3, d(v_5) = 1$$

First Zagreb index for graph 2

 $M_1(G) = \text{ sum of sequence of all vertices}$ $M_1(G) = d^2v_1 + d^2v_2 + d^2v_3 + d^2v_4 + d^2v_5$ $M_1(G) = 2^2 + 3^2 + 3^2 + 1^2 = 4 + 9 + 9 + 1 = 32.$ $Then <math>\frac{M_1(G)}{n} = \frac{32}{5}$ for n = 5 vertices.

Second Zagreb index

$$\begin{split} M_2(g) &= \text{sum of the product of degrees of pair adjacent vertices in molecular graphs.} \\ M_2(g) &= (dv_1 * dv_2) + (dv_2 * dv_3) + (dv_1 * dv_4) + (dv_4 * dv_3) + (dv_2 * dv_4) + (dv_3 * dv_5) \\ M_2(g) &= (3*2) + (3*3) + (3*3) + (3*3) + (3*3) + (3*1) = 6 + 9 + 9 + 9 + 9 = 42 \\ \text{Then } \frac{M_2(G)}{m} &= \frac{42}{6} = 7. \end{split}$$

For graph 3

$$dv_1 = 1, dv_2 = 2, dv_4 = 2, dv_3 = 4, dv_5 = 1$$

First Zagreb index

$$\begin{split} M_1(G) &= \text{ sum of sequence of all vertices} \\ M_1(G) &= d^2v_1 + d^2v_2 + d^2v_3 + d^2v_4 + d^2v_5 = 3^2 + 2^2 + 4^2 + 2^2 + 1^2 = 9 + 4 + 16 + 4 + 1 = 34. \\ \text{Then } \frac{M_1(G)}{n} &= \frac{34}{5} \text{ for } n = 5 \text{ vertices.} \end{split}$$

Second Zagreb index

$$\begin{split} M_2(g) &= \text{sum of the product of degrees of pair adjacent vertices in molecular graphs.} \\ M_2(g) &= (dv_1 * dv_2) + (dv_1 * dv_4) + (dv_2 * dv_3) + (dv_3 * dv_4) + (dv_3 * dv_5) + (dv_1 * dv_5) \\ M_2(g) &= (3*2) + (3*2) + (2*4) + (4*2) + (4*1) + (3*4) = 6 + 6 + 8 + 8 + 4 + 12 = 44. \\ \text{Then } \frac{M_2(G)}{m} &= \frac{44}{6} \text{ Thus the result is true.} \end{split}$$

Let it be true for all the associated bicyclic graphs having pendant vertices less than n. By Lemma 3.2.2 we suppose that there exists a subgraph H such that G-H is an associated bicyclic graph. Let A= {G: $d_G(v_1)=2, d_G(v_i)=1$ for i=2,3... k} and G-H $\notin A$ where |H| is as small as required for H. Here G-H is a subgraph having four vertices or either a pendant vertex with five vertices. We solve this theorem for two cases.

Case1: H is a pendant vertex

Let U=H and V be a neighbor having unique property such that $N_G(V) = \{u, u_1, u_2, \dots, u_k\}$ (k \geq 1). Let G' = G-u where G' is a connected bicycle graph having (n-1) vertices and $G' \notin A$ and then by Mathematical Induction hypothesis such that

 $\frac{M_1(G')}{n-1} \le \frac{M_2(G')}{n} \Rightarrow \frac{32}{5-1} \le \frac{42}{5} \Rightarrow \frac{32}{4} \le \frac{42}{5} \Rightarrow 160 \le 168 \Rightarrow M_1(G') < M_2(G').$ For further details such that $M_1(G) = M_1(G') + 2(K+1) = 160 + 2K + 2 = 2K + 162$ $M_2(G_{-}) = M_2(G') + \sum_{i=1}^k d_G(u_i) + K + 1 \qquad \text{for } \sum_{i=1}^k d_G(u_i) \ge k + 2.$ For $G \notin A$ is a connected bicyclic graph we then further divided this theorem into two cases. Case1(a): $\sum_{i=1}^{k} d_G(u_i) \geq k+3$ Then $\sum_{i=1}^{k} d_{c}(u_{i}) + k + 1 \ge k + 3 + k + 1 = 2k + 4 = 2(k + 2)$ Also, for $M_2(G) = M_2(G') + 2(k+2) = 168+2k+4 = 2k+172=2(k+86)$ For n values $nM_2(G) = n[M_2(G') + \sum_{i=1}^k d_G(u_i) + K + 1]$ $nM_2(G) = nM_2(G') + n(\sum_{i=1}^k d_G(u_i) + K + 1)$ $nM_2(G) = nM_2(G') + n(2k+4)$ $nM_2(G) = nM_2(G') + M_2(G') - GM_2(') + 2nk + 4n$ $nM_2(G) = (n-1)M_1(G') + 2nk + 2n + 2n \odot M_1G(/)/n - 1 < M_2(G')/n$ $> nM_1(G') + 2nk + 2n + M_1(G') + 2k + 2 \odot nM_1(G') \le (n-1)M_2(G')$ $nM_2(G) = (n+1)M_1(G') + 2nk + 2k + 2n + 2 \odot M_1(G) = M_1(G') + 2K + 2 = 2n$ $nM_2(G) = (n+1)M_1(G') + 2k(n+1) + 2(n+1) \odot M_1(G) = M_1(G') + 2(K+1)$ $nM_2(G) = (n+1)M_1(\dot{G}) + (2k+2)(n+1)$ $nM_2(G) \ge (n+1)M_1(G)$ $\frac{M_2(G_{-})}{n+1} > \frac{M_1(G_{-})}{n}$ ⇒ $\frac{M_1(G_{-})}{n} < \frac{M_2(G_{-})}{n}$ *Case 1(b):* Here $\sum_{i=1}^{k} d_G(u_i) \ge k+2$ $d(u_i) = 1$, for i = 1, 2, 3..., k - 1 & $d_G(u_k) = 3$ (i) K≥ 2 Claim that $(M_2G') - (M_1G') > k - 1$

Proof:

Let N $(u_k) = \{v, w_1, w_2\}$ where $d_G(w_2) \ge 2$ for connected bicyclic graphs. Also, if $d_G(w_2) \ge 3$ and $d_G(w_1) \ge 2$ then we suppose that \underline{G} is a connected by bicyclic graph such that $\underline{G} = G' - \bigcup_{i=1}^{k-1} \{u_i\}$ then $\underline{G} \notin A$ for connected bicyclic graph, then by use the result of Mathematical

Induction we have

$$\frac{M_1(\underline{G})}{n-k} \leq \frac{M_2(\underline{G})}{n-k+1} \odot M_1(\underline{G})/n < M_2(\underline{G})/m \Rightarrow M_1(\underline{G}) < M_2(\underline{G}).$$

Moreover, we consider $M_2(G^1) - M_1(G^1) > k-1$ for $d_G(w_3) \ge 2$ then G is connected bicylclic graph. Now we again claim for n times values

$$\begin{split} nM_2(G_{-}) &= (n)M_2(G^1) + \sum_{i=1}^k d_G(v_i)(k+1) = nM_2(G^1) + n(2k+3) = nM_2(G^1) + 2nk + 3n \\ &= nM_2(G^1) - M_2(G^1) + M_2(G^1) + 2nk + 2n + n = (n-1)M_2(G^1) + M_2(G^1) + 2nk + 2n + n \\ &> nM_1(G^1) + M_1(G^1) + k - 1 + 2kn + 2n + (k+3) = M_1(G^1)(n+1) + (n+1)(2k+2) \end{split}$$

$$nM_2(G_{-}) = M_1(G_{-})(n+1)$$

 $M_1(G_{-})/n < M_2(G_{-})/m.$

Similarly, we can prove that

$$M_1(G_3) < M_2(G_3)$$
 for $M_2(G^1) - M_1(G^1) > k - 2$

And

$$M_1(G_4 \) < M_2(G_4) \quad \text{for } M_2(G^1) - M_1(G^1) > k - 2.$$

 $\Rightarrow M_1(G \)/n < M_2(G \)/m.$

which completes proof of theorem. Let us consider extremal tricycle graphs with respect to upper bounds $EM_1(G)$ and lower bounds $EM_2(G)$ respectively as shown in Figure 5.





Theorem 3.2.5: Suppose G be a tricycle graph having order n and such that $EM_1(G) \ge 4n + 68$

having equality hold if $\int_n^1 \in G$. *Proof:*

Let us considered and an associated tricyclic graph we can convert any bicyclic to the tricyclic graph without any pendant vertex as shown in above Figure 5 for i=1,2,3...15 such that

 $EM_i(\alpha_i) = 4n + 68$, for $i = 1, 2, 3, \dots, 5$.

which is the required result.

4. Conclusion

The real fact of this paper is that we have to find external results among the class of bicyclic and tricyclic graphs by using the first and second general Zagreb indices. The first and the second multiplicative Zagreb indices are used for vertex degree-based graphs [22-24] with the given diameter among different classes of bicycle and tricycle graphs respectively. This paper is grateful to help the readers about different types of bicyclic and tricyclic graphs and comparing their results by using the property of bounds by using methods of Zagreb indices as well.

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