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COMPARISON OF NOVEL INDEX WITH GEOMETRIC−ARITHMETIC AND SUM−CONNECTIVITY INDICES

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Abstract. This work focusses on the minimal, second minimal, maximal and second maximal values of three indices for various unicyclic, bicyclic graphs. Motivated by the works of Ghorbani, this work compares the extremal values among three indices viz., geometric−arithmetic, sum−connectivity and proposed novel index (geometric−harmonic) and these indices are computed for star, cycle and path. Relations are established among the indices for star, cycle, path, tree, complete, unicyclic and bicyclic graphs.

Keywords: geometric−arithmetic index; sum−connectivity index; geometric−harmonic index.

2010 AMS Subject Classification: 05C05, 05C07, 05C35, 05C38.

1. Introduction

In this paper, the graphs considered are simple and loop free. A graph is a collection of vertices and edges, where edge is a link between two vertices. The degree of a vertex is the number of edges incident to that vertex. The path is a sequence of vertices placed adjacent to

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each other and joined using edges. A connected graph is one which has a path from any point to any other point in the graph. A graph which exactly depicts like a star in which a central node p is connected to $p-1$ pendant edges is a star graph. The degree of the central node will be $p-1$ and the degree of the $p-1$ edges will be unity.

A complete graph is a graph in which each pair of graph vertices is connected by an edge. The complete graph with n vertices has $n(n-1)/2$ number of edges. A cycle is a connected graph with all vertices of degree 2. If n vertices are considered in a cycle C_n, then there are n edges in the cycle C_n [4].

The graph theory has its use in almost every fields [2, 5, 6, 7, 8, 10, 14] and it plays a significant role in mathematical chemistry for drawing the information of a chemical compound and also in the design of drugs. Robust methods and a large database are available for designing drugs. Survey relating the molecular structure to a particular property using tools of statistics are very significant. This is often referred to as QSPR and QSAR studies [1, 11, 12, 15, 16, 18]. The structure in which the atoms are bonded to each other are very important in order to carry out the study on it. The structure of the compound is a treasure of information of the respective compound. A two-dimensional descriptor that considers the arrangement of compounds, size, shape, branching etc, conceals the information in numerical form. Topological indices play a key role in the applications of the compounds in QSAR and QSPR studies [3, 9, 13, 17, 19, 21]. In this work, we discuss the extremal values of three indices and establish relations among them.

2. PRELIMINARIES

Vukicevic et al., [20] designed a topological index called geometric−arithmetic index is the ratio of geometric mean of end vertex degrees of an edge uv to arithmetic mean of end vertex degrees of the edge uv and is defined as

$$GA(G) = \sum \frac{2\sqrt{d_u.d_v}}{d_u + d_v}$$

where (u,v) is an element of $E(G)$.

Zhou et al., [22] introduced the sum−connectivity index and is defined as

$$\chi(G) = \sum \frac{1}{\sqrt{d_u + d_v}}$$

where (u,v) *is an element of* $E(G)$.

Motivated by Vukicevic in designing GA index, an attempt to design a new degree based index geometric−harmonic index is made and introduced as the ratio of geometric mean of end vertex degrees of an edge *uv* to harmonic mean of end vertex degrees of the edge *uv*. It is defined as

$$GH(G) = \sum \frac{(d_u + d_v)\sqrt{d_u.d_v}}{2}$$

where (u,v) *is an element of* $E(G)$.

This index is computed and comparison of all the above defined three indices for unicyclic and bicyclic graphs are carried out.

3. Main Results

Theorem 3.1. *Suppose* S_n *be the star graph on n vertices. The degree of the central vertex is* $(n-1)$ *and others are pendant vertices. Then the above discussed three indices are given by*

$$GA(S_n) = \frac{2(n-1)^{\frac{3}{2}}}{n}.$$

$$\chi(S_n) = \frac{(n-1)}{\sqrt{n}}.$$

$$GH(S_n) = \frac{n(n-1)^{\frac{3}{2}}}{2}.$$

Proof. The proof is trivial. □

Theorem 3.2. *Let* K_n *be a complete graph with n vertices. Then the indices are respectively given by*

$$GA(K_n) = \frac{n(n-1)}{2}.$$

$$\chi(K_n) = \frac{n\sqrt{(n-1)}}{2\sqrt{2}}.$$

$$GH(K_n) = \frac{n(n-1)^3}{2}.$$

Proof. The proof is trivial. □

Theorem 3.3. *Consider a path P_n with n vertices. Then the indices are respectively given by*

$$GA(P_n) = \frac{4\sqrt{2}}{3} + (n-3).$$

$$\chi(P_n) = \frac{(n-2)}{2} + \frac{2}{\sqrt{3}}.$$

$$GH(P_n) = 4n + (3\sqrt{2} - 12).$$

Proof. The proof is trivial. □

Theorem 3.4. *Let C_n be a cycle with n vertices and each vertex degree is 2. Then the indices are respectively given by*

$$GA(C_n) = n.$$

$$\chi(C_n) = \frac{n}{2}.$$

$$GH(C_n) = 4n.$$

Proof. The proof is trivial. However, an interesting point to note in this particular case is that, the three indices for a cycle C_n are related as

$$\chi(C_n) = \frac{GA(C_n)}{2}.$$

$$GH(C_n) = 4GA(C_n).$$

$$GH(C_n) = 8\chi(C_n).$$

□

Theorem 3.5. *Let G be any connected graph with n vertices. Then the indices take the expression*

$$GA(G) \leq GA(K_n).$$

$$\chi(G) \leq \chi(K_n).$$

$$GH(G) \leq GH(K_n).$$

Proof. As the complete graph has $n(n-1)/2$ number of edges of degree $(n-1, n-1)$, the topological index will be larger for complete graph compared to any simple graph G.
The proof is trivial. □

Theorem 3.6. *A tree with n vertices with minimal GA index is a star S_n. The GA index of S_n is given by*

$$GA(S_n) = \frac{2(n-1)^{\frac{3}{2}}}{n}.$$

where $n \geq 4$

Proof. Consider a star $n \geq 4$ for which one vertex is of degree $(n-1)$ and the rest $(n-1)$ vertices are pendant vertices. A star S_n has $(n-1)$ edges and end degree vertices are $(n-1)$ and 1 respectively. Then using GA index of star graph is

$$GA(S_n) = \frac{2(n-1)^{\frac{3}{2}}}{n}.$$

Thus, it is clear that any tree of vertices $n \geq 4$ has GA index more than that of a star graph. □

Theorem 3.7. *The minimal GA index and minimal sum−connectivity index of a n−vertex connected unicyclic graph is $(S_n + e)$ and is given by*

$$GA(S_n+e) = \frac{2(n-3)(n+1)\sqrt{n-1} + n(n+1) + 4n\sqrt{(2n-2)}}{n(n+1)}.$$

$$\chi(S_n+e) = \frac{(n-3)}{\sqrt{n}} + \frac{1}{2} + \frac{2}{\sqrt{(n+1)}}.$$

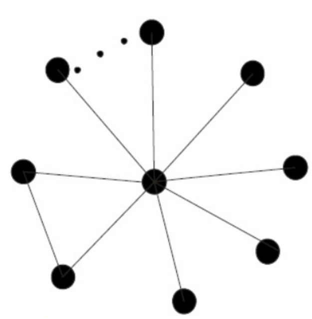

FIGURE 1. The Graph $S_n + e$.

Proof. Any n−vertex connected unicyclic graph has GA index and sum−connectivity index more than that of a graph in $Fig.1$. The graph as shown in $Fig.1$ has $(n-3)$ edges of $(1, n-1)$, 1 edge of $(2,2)$ and 2 edges of $(2,n-1)$ types. Using all these vertices and edges and definition of *GA* index and sum−connectivity index, we arrive at the results.

$$GA(S_n+e) = \frac{2(n-3)(n+1)\sqrt{n-1}+n(n+1)+4n\sqrt{2n-2}}{n(n+1)}.$$

$$\chi(S_n+e) = \frac{(n-3)}{\sqrt{n}} + \frac{1}{2} + \frac{2}{\sqrt{(n+1)}}.$$

□

Theorem 3.8. *Among all the unicyclic graphs on n vertices, the graph S_n+e has the maximal geometric−harmonic index. The geometric−harmonic index for this graph is*

$$GH(S_n+e) = \frac{n(n-3)\sqrt{n-1}}{2} + 4 + (n+1)\sqrt{2n-2}.$$

Proof. From the $Fig.1$ considering the total number of edges with its respective end vertices, the *GH* index results in

$$GH(S_n+e) = \frac{n(n-3)\sqrt{n-1}}{2} + 4 + (n+1)\sqrt{2n-2}.$$

□

Theorem 3.9. *The minimal GA index among all bicyclic graphs is for the graph depicted in $Fig.2$. This is given by*

$$GA(G) = 2\frac{(n-4)\sqrt{(n-1)}}{n} + 4\frac{\sqrt{(2n-2)}}{(n+1)} + \frac{2\sqrt{(3n-3)}}{(n+2)} + \frac{4\sqrt{6}}{5}.$$

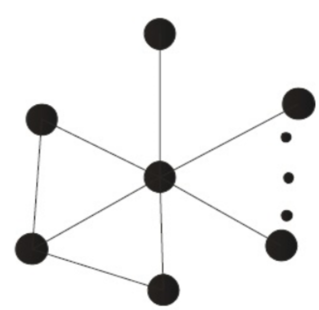

FIGURE 2. The Graph G.

Proof. The graph G depicted in $Fig.2$ has $(n-4)$ edges of $(1,n-1)$, 2 edges of $(2,n-1)$, 1 edge of $(3,n-1)$ and 2 edges of $(2,3)$ types. Considering the total number of edges with its respective end vertices, the GA index results in

$$GA(G) = 2\frac{(n-4)\sqrt{(n-1)}}{n} + 4\frac{\sqrt{(2n-2)}}{n+1} + \frac{2\sqrt{3n-3}}{n+2} + \frac{4\sqrt{6}}{5}.$$

It is found that GA index is the minimal for the graph G as shown in $Fig.2$ among n−vertex connected bicyclic graphs. □

Theorem 3.10. *The minimal sum−connectivity index (only for $n \leq 10$) among all bicyclic graphs, is for the graph in $Fig.2$. It is given by*

$$\chi(G) = \frac{n-4}{\sqrt{n}} + \frac{2}{\sqrt{n+1}} + \frac{1}{\sqrt{n+2}} + \frac{2}{\sqrt{5}}.$$

Proof. From the $Fig.2$ considering the total number of edges with its respective end vertices, the sum−connectivity index results in

$$\chi(G) = \frac{n-4}{\sqrt{n}} + \frac{2}{\sqrt{n+1}} + \frac{1}{\sqrt{n+2}} + \frac{2}{\sqrt{5}}.$$

It is found that the sum−connectivity index is the minimal for a graph G as shown in $Fig.2$ among n−vertex connected bicyclic graphs. □

Theorem 3.11. *The maximal geometric−harmonic index in all bicyclic graphs is for the graph G depicted in the graph $Fig.2$. The value of the index for the graph G is*

$$GH(G) = \frac{n(n-4)\sqrt{n-1} + 2(n+1)\sqrt{2n-2} + (n+2)\sqrt{3n-3} + 10\sqrt{6}}{2}.$$

Proof. From the $Fig.2$ considering the total number of edges with its respective end vertices, the GH index results in

$$GH(G) = \frac{n(n-4)\sqrt{n-1} + 2(n+1)\sqrt{2n-2} + (n+2)\sqrt{3n-3} + 10\sqrt{6}}{2}.$$

□

Theorem 3.12. *The second minimal GA index among all unicyclic graphs is for the graph in $Fig.3$. It is given by*

$$GA(S_n + e + e') = \frac{2(n-4)\sqrt{n-2}}{n-1} + \frac{4\sqrt{2n-2}}{n} + 2.$$

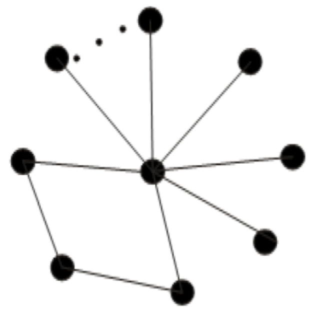

FIGURE 3. The Graph S_n+e+e'.

Proof. The graph S_n+e+e' depicted in the $Fig.3$ has $(n-4)$ edges of $(n-2,1)$, 2 edges of $(2,n-2)$ and 2 edges of $(2,2)$ types. Considering the total number of edges with its respective end vertices, the GA index results in

$$GA(S_n+e+e') = \frac{2(n-4)\sqrt{n-2}}{n-1} + \frac{4\sqrt{2n-2}}{n} + 2.$$

It is found that the GA index is the second minimal for a graph S_n+e+e' as shown in $Fig.3$ among n−vertex connected unicyclic graphs.

□

Theorem 3.13. *The second minimal sum−connectivity index among all unicyclic graphs is for the graph in $Fig.3$. It is given by*

$$\chi(S_n+e+e') = \frac{n-4}{\sqrt{n-1}} + \frac{2}{\sqrt{n}} + 1.$$

Proof. From the $Fig.3$ considering the total number of edges with its respective end vertices, the sum−connectivity index results in

$$\chi(S_n+e+e') = \frac{n-4}{\sqrt{n-1}} + \frac{2}{\sqrt{n}} + 1.$$

It is found that the sum−connectivity index is the second minimal for a graph S_n+e+e' as shown in $Fig.3$ among n−vertex connected unicyclic graphs.

□

Theorem 3.14. *The second maximal GH index among all unicyclic graphs is for the graph in $Fig.3$. It is given by*

$$GH(S_n+e+e') = \frac{(n-4)(n-1)\sqrt{n-2} + 2n\sqrt{2n-4} + 16}{2}.$$

Proof. From the *Fig*.3 considering the total number of edges with its respective end vertices, the GH index results in

$$GH(S_n+e+e') = \frac{(n-4)(n-1)\sqrt{n-2}+2n\sqrt{2n-4}+16}{2}.$$

It is found that the GH index is the second maximal for a graph S_n+e+e' as shown in *Fig*.3 among n−vertex connected unicyclic graphs. □

Theorem 3.15. *The n−vertex tree with maximal GA index is the path P_n in which $GA(T) < GA(P_n)$. The GA index of a path P_n is given in the previous results.*

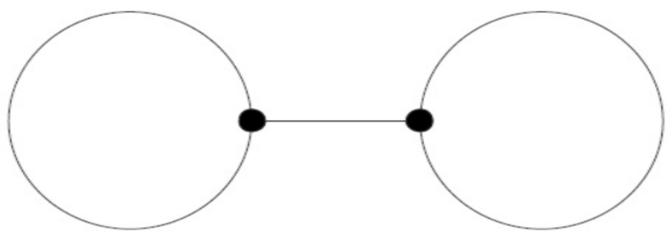

FIGURE 4. The Graph H.

Proof. The graph H is a n−vertex bicyclic and connected graph. It has n vertices and $n+1$ edges. The graph in the *Fig*.4 has 4 edges of $(2,3)$, 1 edge of $(3,3)$ and $n-4$ edges of $(2,2)$ types. GA index is the maximal for the graph H among bicyclic graphs. The GA index results in

$$GA(H) = n-3+\frac{8\sqrt{6}}{5}.$$

□

Theorem 3.16. *Among all bicyclic graphs on n vertices, the graph H in Fig.4 has the second maximal sum−connectivity index and it is given by*

$$\chi(H) = \frac{4}{\sqrt{5}}+\frac{1}{3}+\frac{n-4}{2}.$$

Proof. From the *Fig*.4 considering the total number of edges with its respective end vertices, the sum−connectivity index results in

$$\chi(H) = \frac{4}{\sqrt{5}}+\frac{1}{3}+\frac{n-4}{2}.$$

It is found that sum−connectivity index is the second maximal for the graph H as shown in $Fig.4$ among connected bicyclic graphs. □

Theorem 3.17. *Among all bicyclic graphs on n vertices, the graph H in $Fig.4$ has minimal GH index and it is given by*

$$GH(H) = 4n + 10\sqrt{6} - 12.$$

Proof. From the $Fig.4$ considering the total number of edges with its respective end vertices, the GH index results in

$$GH(H) = 4n + 10\sqrt{6} - 12.$$

It is found that GH index is the minimal for the graph H as shown in $Fig.4$ among connected bicyclic graphs. □

Theorem 3.18. *The n−vertex connected tree with second minimal GA index is the graph $(S_n)'$. The GA index of $(S_n)'$ is*

$$GA(S_n)' = \frac{2(n-3)\sqrt{n-2}}{n-1} + \frac{2\sqrt{2n-4}}{n} + \frac{2\sqrt{2}}{3}.$$

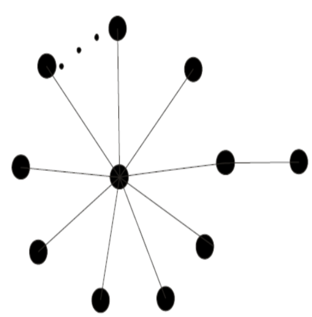

FIGURE 5. The Graph S_n'.

Proof. The graph $(S_n)'$ has n vertices and $n-1$ edges. The $(S_n)'$ has $n-3$ edges of $(n-2,1)$, 1 edge of $(n-2,2)$ and 1 edge of $(1,2)$ types. Using GA index for $(S_n)'$, we get the required result and found to be the second minimal among the trees. □

Theorem 3.19. *The n−vertex connected tree with minimal GH index is the graph $(S_n)'$. The GH index of $(S_n)'$ is*

$$GH(S_n)' = \frac{(n^2-4n+3)\sqrt{n-2} + n\sqrt{2n-4} + 3\sqrt{2}}{2}.$$

Proof. From the *Fig*.5 considering the total number of edges with its respective end vertices, the *GH* index results in

$$GH(S_n)' = \frac{(n^2-4n+3)\sqrt{n-2}+n\sqrt{2n-4}+3\sqrt{2}}{2}.$$

□

Theorem 3.20. *Among all bicyclic graphs on n vertices, the graph F in Fig.6 has the second minimal GA index and is given by*

$$GA(F) = \frac{2(n-5)\sqrt{n-2}}{n-1} + \frac{4\sqrt{2n-4}}{n} + \frac{2\sqrt{3n-6}}{n+1} + \frac{4\sqrt{6}}{5} + 1.$$

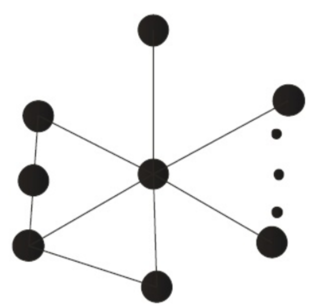

FIGURE 6. The Graph F.

Proof. In graph F, n−vertex connected bicyclic graph, there are $n+1$ edges. There are $n-5$ edges of $(1,n-2)$, 2 edges of $(2,n-2)$, 1 edge of $(3,n-2)$, 2 edges of $(2,3)$ and 1 edge of $(2,2)$ types in graph F. $GA(F)$ results in the following formula by using above edges and found to be second minimal among all bicyclic graphs. Hence follows the result.

$$GA(F) = \frac{2(n-5)\sqrt{n-2}}{n-1} + \frac{4\sqrt{2n-4}}{n} + \frac{2\sqrt{3n-6}}{n+1} + \frac{4\sqrt{6}}{5} + 1.$$

□

Theorem 3.21. *Among all bicyclic graphs for n vertices, the graph F in Fig.6 has the second minimal sum−connectivity index and is given by*

$$\chi(F) = \frac{n-5}{\sqrt{n-1}} + \frac{2}{\sqrt{n}} + \frac{1}{\sqrt{n+1}} + \frac{2}{\sqrt{5}} + \frac{1}{2}.$$

Proof. From the $Fig.6$ considering the total number of edges with its respective end vertices, the sum−connectivity index results in

$$\chi(F) = \frac{n-5}{\sqrt{n-1}} + \frac{2}{\sqrt{n}} + \frac{1}{\sqrt{n+1}} + \frac{2}{\sqrt{5}} + \frac{1}{2}.$$

□

Theorem 3.22. *Among all bicyclic graphs for $n \leq 10$ vertices, the graph F in $Fig.6$ has the second maximal GH index and is given by*

$$GH(F) = \frac{(n^2-6n+5)\sqrt{n-2} + 2n\sqrt{2n-4} + (n+1)\sqrt{3n-6} + 10\sqrt{6} + 8}{2}.$$

Proof. From the $Fig.6$ considering the total number of edges with its respective end vertices, the GH index results in

$$GH(F) = \frac{(n^2-6n+5)\sqrt{n-2} + 2n\sqrt{2n-4} + (n+1)\sqrt{3n-6} + 10\sqrt{6} + 8}{2}.$$

It is found that the GH index is the second maximal for a graph F as shown in $Fig.6$ among all bicyclic graphs.

□

Theorem 3.23. *The $n-$vertex tree with maximal GA index, sum−connectivity index and GH index is the graph Q in $Fig.7$. It is given by*

$$GA(Q) = n - 6 + \frac{4}{\sqrt{3}} + \frac{4\sqrt{6}}{5} + \frac{\sqrt{3}}{2}.$$

$$\chi(Q) = \frac{n-6}{2} + \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{5}} + \frac{1}{2}.$$

$$GH(Q) = \frac{8(n-6) + 6\sqrt{2} + 10\sqrt{6} + 4\sqrt{3}}{2}.$$

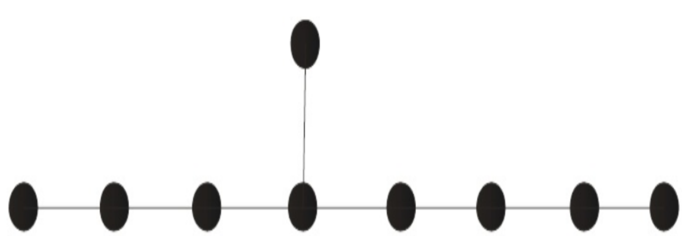

FIGURE 7. The Graph Q.

Proof. The graph Q has n vertices and $n-1$ edges. There are $n-6$ edges of $(2,2)$, 2 edges of $(1,2)$, 2 edges of $(2,3)$ and 1 edge of $(1,3)$ types in graph Q. The number of edges are considered and GA index, sum$-$connectivity index and GH index are found to be maximal for the graph Q. It is obtained as

$$GA(Q) = n-6+\frac{4}{\sqrt{3}}+\frac{4\sqrt{6}}{5}+\frac{\sqrt{3}}{2}.$$

$$\chi(Q) = \frac{n-6}{2}+\frac{2}{\sqrt{3}}+\frac{2}{\sqrt{5}}+\frac{1}{2}.$$

$$GH(Q) = \frac{8(n-6)+6\sqrt{2}+10\sqrt{6}+4\sqrt{3}}{2}.$$

□

Theorem 3.24. *The $n-$vertex connected unicyclic graph with second maximal GA and sum$-$connectivity index is graph R, depicted in Fig.8. It is given by*

$$GA(R) = n-4+\frac{2\sqrt{2}}{3}+\frac{6\sqrt{6}}{5}.$$

$$\chi(R) = \frac{n-4}{2}+\frac{1}{\sqrt{3}}+\frac{3}{\sqrt{5}}.$$

The GA index of graph R and C_n are related by

$$GA(R) = GA(C_n) - 0.11779.$$

The sum$-$connectivity index of graph R and C_n are related by

$$\chi(R) = \chi(C_n) - 0.0810.$$

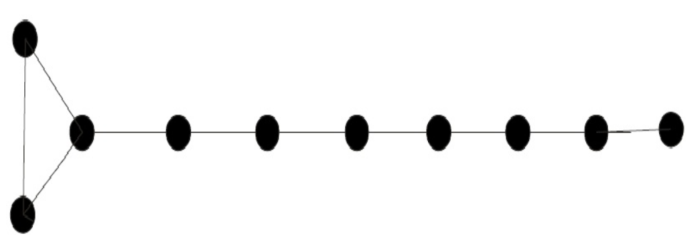

FIGURE 8. The Graph R.

Proof. The graph R in Fig.8 has n vertices and n edges. The edges found in graph R are $n-4$ of $(2,2)$, 1 of $(1,2)$ and 3 of $(2,3)$ types. Using this data, the results are as follows. It is found that among the n−vertex connected unicyclic graphs, graph R has the second maximal GA index and sum−connectivity index. It is clear by the relation that GA index of graph R reduces by a quantity of 0.11779 compared to the GA index of C_n among all unicyclic graphs. It is clear by the relation that sum−connectivity index of graph R reduces by a quantity of 0.0810 compared to the sum−connectivity index of C_n among all unicyclic graphs.

$$GA(R) = GA(C_n) - 0.11779.$$

$$\chi(R) = \chi(C_n) - 0.0810.$$

□

Theorem 3.25. *The n−vertex connected unicyclic graph with second minimal GH index is graph R, depicted in $Fig.8$. It is given by*

$$GH(R) = \frac{8(n-4) + 3\sqrt{2} + 15\sqrt{6}}{2}.$$

The GH index of graph R and C_n are related by

$$GH(R) = GH(C_n) + 4.4923.$$

Proof. The graph R in $Fig.8$ has n vertices and n edges. The edges found in graph R are $n-4$ of $(2,2)$, 1 of $(1,2)$ and 3 of $(2,3)$ types. Using this data, the results are as follows. It is found that among the n−vertex connected unicyclic graphs, graph R has the second minimal GH index and it is clear by the relation that GH index of graph R increases by a quantity 4.4923 compared to the GH index of C_n among all unicyclic graphs. □

Theorem 3.26. *Among the bicyclic graphs on n vertices, the graph S in $Fig.9$ has the second maximal GA index and the sum−connectivity index is maximal and the GH index is second minimal$(n \geq 12)$ for the bicyclic graph S and are given by*

$$GA(S) = n - 5 + \frac{12\sqrt{6}}{5}.$$

$$\chi(S) = \frac{n-5}{2} + \frac{6}{\sqrt{5}}.$$

$$GH(S) = \frac{8(n-5) + 30\sqrt{6}}{2}.$$

The relation of GA index for the graphs S and H is given by

$$GA(S) = GA(H) - 0.040408.$$

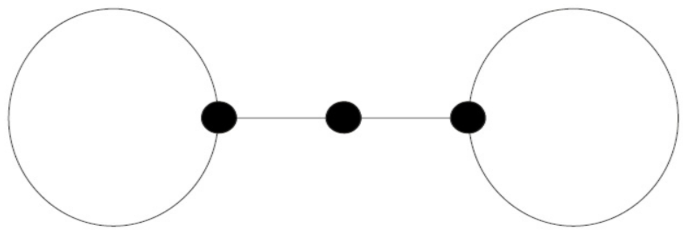

FIGURE 9. The Graph S.

Proof. The graph S is a bicyclic n$-$vertex connected graph with $n+1$ edges. There are $n-5$ edges of $(2,2)$ and 6 edges of $(2,3)$ types. The GA index follows as above. It is found to be the second maximal among bicyclic graphs. The GA index of the graph S is second maximal when compared to the GA index of the graph H as GA index of the graph S reduces by a quantity 0.040408 to that of GA index of the graph H. The sum$-$connectivity index is found to be maximal among all bicyclic graphs considered in this study. The GH index is minimal for the bicyclic graph S up to $n \leq 9$ and it is second minimal as $n \geq 12$. Hence,

$$GA(S) = n - 5 + \frac{12\sqrt{6}}{5}.$$
$$\chi(S) = \frac{n-5}{2} + \frac{6}{\sqrt{5}}.$$
$$GH(S) = \frac{8(n-5) + 30\sqrt{6}}{2}.$$
$$GA(S) = GA(H) - 0.040408.$$

□

4. CONCLUSION

In this study the extremal values of unicyclic and bicyclic graphs using three indices viz., geometric-arithmetic(GA), sum-connectivity(χ), geometric-harmonic(GH) are computed. A novel topological index known as geometric-harmonic index is introduced and relations are established among the indices for star, cycle, path, tree, complete, unicyclic and bicyclic graphs using other two indices considered under the study.

CONFLICT OF INTERESTS

The author(s) declare that there is no conflict of interests.

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