

Sharp upper bounds on forgotten and SK indices of cactus graph

Ammar Alsinai *

*Department of Studies in Mathematics
University of Mysore, Manasagangotri
Mysuru 570006
Karnataka
India*

Hafiz Mutee ur Rehman [†]

Yasir Manzoor [§]

*Department of Mathematics
Division of Science and Technology
University of Education
Lahore
Pakistan*

Murat Cancan [‡]

*Faculty of Education
Van Yuzuncu Yıl University
Zeve Campus
Tuşba, 65080
Van
Turkey*

Ziyattin Taş [@]

*Department of Mathematics
Bingöl University
Turkey*

* E-mail: aliiammr1985@gmail.com (Corresponding Author)

† E-mail: mutee.rehman@ue.edu.pk

§ E-mail: yasir36402@gmail.com

‡ E-mail: m_cencen@yahoo.com, mcancan@yyu.edu.tr

@ E-mail: ztas@bingol.edu.tr

Moahmmad Reza Farahani [#]

Department of Mathematics

Iran University of Science and Technology (IUST)

Narmak

Tehran 16844

Iran

Abstract

Sheehalli and Kanabur presented new forms of topological indices known as *SK* indices which have many applications in chemical graph theory towards *QSPR/QSAR*. A simple connected graph Γ is called a cactus graph if and only if any two cycles in the graph have no common edge. In this paper, we will explore and determine the sharp upper bounds of cactus graph using different versions of *SK* indices. We will also characterize the extremal properties for these indices due to many applications in pharmacology and medicinal chemistry.

Subject Classification: Primary 05C31, 92E10.

Keywords: Topological index, Chemical graph theory, Cactus graph.

1. Introduction

Graph theory is the most fundamental approach [1-4], which is applicable in computer sciences [5], data mining [6], job and time table scheduling [7, 8], game theory etc. Computer networking provides a technique of communication between a number of processors connected in a network.

During recent decades molecular topology, mathematical chemistry and applied graph theory have become the important area of research. In the field of molecular graphs [12], representation of the atoms is as vertices and bonds as edges. The numerical representation of the molecule graph as a single number, is usually called topological index. Readers can see the paper series [29-39].

Let $\Gamma = (V, E)$ be a graph, where V is the set of vertices and E represents the set of edges of the graph Γ , similarly $T = (V, E)$ be a tree and $|\Gamma| = n$ gives the total number of vertices in graph Γ . In this paper, we are concerned with all graphs which are finite, simple, connected, undirected and non weighted. The degree of a vertex $u \in V$ in a graph Γ is the number of vertices adjacent to the vertex u in Γ , and is denoted as $d_{\Gamma}(u)$.

[#] E-mail: Mohammad_Farahani@mathdep.iust.ac.ir, Mrfarahani88@gmail.com

Wiener was first to introduce the first degree based topological index [9] which was used to determine the boiling point of paraffin. Till now hundredth of topo-logical indices are introduced. In [10] different versions of degree based topological indices were presented.

One of the oldest and most considered index is Zagreb index which was introduced by Gutman [15, 28] and Trinajstić [11]. Due to the more predictive ability towards QSPR different versions of degree based topological indices were introduced in [19, 26, 27] and are called SK and SK_1 indices and are defined as:

$$SK(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{d(u) + d(v)}{2}, SK_1(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{d(u)d(v)}{2}, SK_2(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{(d(u) + d(v))^2}{4}.$$

In 2015 Fortula and Gutman introduced forgotten index in [15], which is given as:

$$F(\Gamma) = \sum_{uv \in E(\Gamma)} (d_u(u)^2 + d_v(v)^2) = \sum_{u \in V(\Gamma)} d_u(u)^3.$$

If $M_1(\Gamma)$, $M_2(\Gamma)$, $F(\Gamma)$ are first Zagreb, second Zagreb and forgotten indices then one can write

$$SK(\Gamma) = \frac{M_1(\Gamma)}{2}, SK_1(\Gamma) = \frac{M_2(\Gamma)}{2}, SK_2(\Gamma) = \frac{1}{4}F(\Gamma) + SK_1(\Gamma).$$

An undirected connected graph is called cactus graph if any two cycles in the graph does not have common edge. In an undirected connected graph, a cut vertex is a vertex whose removal results into a disconnected graph. A block is a maximal subgraph without a cut-vertex. If every block in graph is an edge or a cycle then graph is cactus graph. The Figure 1 is the natural representation of cactus tree or graph in which there are cycles and thorns are representing the pendent vertices.

Since a cactus graph (Figure 2) may have some pendent vertices then a set C_n^k is the set of cactus graphs with k pendent vertices and n is total number of vertices such that $n \geq k \geq 0$. A pendent edge is an edge which have one pendent vertex. For $i \geq 1$, let $P_1 = \{\rho_1, \rho_2, \rho_3, \dots, \rho_p, \rho'1\}$, $P_2 = \{\rho_1, \rho_2, \rho_3, \dots, \rho_p, \rho'2\}, \dots, P_r = \{\rho_1, \rho_2, \rho_3, \dots, \rho_p, \rho'r\}$ are the paths of a graph Γ such that there exist atmost one cycle C such that $V(P_i) \cap V(C) = \{u_i\}$ and $d_v u_i = 1$, $i \geq 1$, then the induced subgraph $\Gamma(\{\rho'_i, \rho_j, i \in (1, r), j \in (1, p)\})$ is called dense path. In particularly when $r = 1$ the dense path becomes pendent path. The length of dense path is equal to the length of its pendent path. Cauchy-Schwarz inequality states that for all sequences of real numbers u_i and v_i , we have



Figure 1
Cactus Graph in Nature.

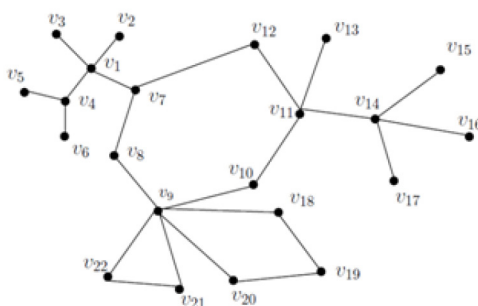


Figure 2
Cactus Graph.

$$\left(\sum_{i=1}^n u_i^2 \right) \left(\sum_{i=1}^n v_i^2 \right) \geq \left(\sum_{i=1}^n u_i v_i \right)^2.$$

Equality holds if $u_i = kv_i$ for a non-zero constant $k \in \mathbb{R}$. Also equality holds when we put $v_i = 1$ then $u_1 = u_2 = u_3 = \dots = u_n$.

Wang discussed the extremality of cactus graph using multiplicative Zagreb in-dices in [14]. Some results on lower bounds using topological indices are given in [16]. Ravi et al., calculated SK indices for the graphene structure based on the neighborhood degree obtain results based on both sum and products of the cardinality of edge partitions corresponding to four different Graphene structures in [23]. SK indices of conical graph were also discussed by Alameri et al., in [24]. Rajini et al., gave SK Indices of Graph Operator $S(G)$ and $R(G)$ on few nano structures in [27].

In the present article, we aim to study sharp upper bounds on forgotten $F(\Gamma)$ and SK Indices of cactus graph Γ , we also characterize the extremal properties for given class of graphs.

2. Extremal SK Indices of Cactus graph

2.1 Main Results

In this section we discuss some preliminary lemmas which are used to prove our theorems. Let $\Gamma \in \mathcal{C}^k$ be a graph then by using the definitions of $SK(\Gamma)$, $SK_1(\Gamma)$, and $SK_2(\Gamma)$, we have following results:

Lemma 2.1 : Let d_u and d_v are the degrees of any two vertices of a connected graph Γ such that $d_u \geq d_v$. Suppose that $N(u)/N(v) = \{u_1, u_2, \dots, u_k\}$, $N(v)/N(u) = \{v_1, v_2, \dots, v_h, v_{h+1}, \dots, v_l\}$, $1 \leq l \leq d_v$ with $\sum_{i=1}^k d_{u_i} \geq \sum_{i=h+1}^l d_{v_i}$, then there exist a new graph $\Gamma' = (\Gamma - \{v_1 v_2 v_3, \dots, v_h v\}) \cup \{v_1 u, v_2 u, \dots, v_h u\}$ and

1. If $uv \in E(\Gamma)$ then $SK_1(\Gamma') \geq SK_1(\Gamma)$;
2. If $uv \notin E(\Gamma)$ then $SK_1(\Gamma') > SK_1(\Gamma)$.

Proof : Suppose that, for convenience, $N(u) \cap N(v) = \{v_{l+1}, v_{l+2}, \dots, v_{d_v}\}$. If $uv \in E(\Gamma)$, by using the definition of SK_1 index

$$\begin{aligned} SK_1(\Gamma') - SK_1(\Gamma) &= \frac{1}{2} (d_{\Gamma'}(u) \sum_{i=l+1}^{d_v} d_{\Gamma'}(v_i) + d_{\Gamma'}(u) \sum_{i=1}^k d_{\Gamma'}(u_i) \\ &\quad + d_{\Gamma'}(u) \sum_{i=1}^h d_{\Gamma'}(v_i) + d_{\Gamma'}(v) \sum_{i=h+1}^{d_v} d_{\Gamma'}(v_i) + d_{\Gamma'}(u) d_{\Gamma'}(v) \\ &\quad - d_{\Gamma}(v) \sum_{i=1}^{d_v} d_{\Gamma}(v_i) - d_{\Gamma}(u) \sum_{i=l+1}^{d_v} d_{\Gamma}(v_i) - d_{\Gamma}(u) \sum_{i=1}^k d_{\Gamma}(u_i) - d_{\Gamma}(u) d_{\Gamma}(v) \end{aligned}$$

$$\text{And } d_{\Gamma'}(v) - d_{\Gamma}(v) = h, d_{\Gamma'}(u) - d_{\Gamma}(u) = h$$

Then

$$\begin{aligned} SK_1(\Gamma') - SK_1(\Gamma) &= \frac{1}{2} ((k+h-l) \sum_{i=1}^h d_{\Gamma}(v_i) + h (\sum_{i=1}^k d_{\Gamma}(u_i) - \sum_{i=h+1}^l d_{\Gamma}(v_i)) \\ &\quad + (k+h)(l-h) - (k)(l)) \\ SK_1(\Gamma') - SK_1(\Gamma) &\geq \frac{1}{2} ((k+h-l)h + h (\sum_{i=1}^k d_{\Gamma}(u_i) - \sum_{i=h+1}^l d_{\Gamma}(v_i)) \\ &\quad + (k+h)(l-h) - (k)(l)) \end{aligned}$$

$$SK_1(\Gamma') - SK_1(\Gamma) \geq \frac{1}{2} (h(\sum_{i=1}^k d_{\Gamma}(u_i) - \sum_{i=h+1}^l d_{\Gamma}(v_i)))$$

$$SK_1(\Gamma') - SK_1(\Gamma) \geq 0$$

This inequality holds if $\sum_{i=1}^k d_{\Gamma}(u_i) \geq \sum_{i=h+1}^l d_{\Gamma}(v_i)$. Therefor $SK_1(\Gamma') \geq SK_1(\Gamma)$ which gives the contradiction to the choice of Γ .

(2) If $uv \notin E(\Gamma)$, by using the definition of SK_1 index

$$\begin{aligned} SK_1(\Gamma') - SK_1(\Gamma) = & \frac{1}{2} (d_{\Gamma'}(u) \sum_{i=l+1}^{d_v} d_{\Gamma}(v_i) + d_{\Gamma'}(u) \sum_{i=1}^k d_{\Gamma}(u_i) + d_{\Gamma'}(u) \sum_{i=1}^h d_{\Gamma}(v_i) \\ & + d_{\Gamma'}(v) \sum_{i=h+1}^{d_v} d_{\Gamma}(v_i) - d_{\Gamma}(v) \sum_{i=1}^{d_v} d_{\Gamma}(v_i) - d_{\Gamma}(u) \sum_{i=l+1}^{d_v} d_{\Gamma}(v_i) - d_{\Gamma}(u) \sum_{i=1}^k d_{\Gamma}(u_i)) \end{aligned}$$

Now, by using the above equations

$$\begin{aligned} SK_1(\Gamma') - SK_1(\Gamma) = & \frac{1}{2} ((d_{\Gamma'}(u) - d_{\Gamma}(v)) \sum_{i=1}^h d_{\Gamma}(v_i) + h(\sum_{i=1}^k d_{\Gamma}(u_i) \\ & - \sum_{i=h+1}^l d_{\Gamma}(v_i))) SK_1(\Gamma') - SK_1(\Gamma) > \frac{1}{2} ((d_{\Gamma'}(u) - d_{\Gamma}(v)) \sum_{i=1}^h d_{\Gamma}(v_i) \\ & + h(\sum_{i=1}^k d_{\Gamma}(u_i) - \sum_{i=h+1}^l d_{\Gamma}(v_i))) SK_1(\Gamma') - SK_1(\Gamma) \geq 0 \end{aligned}$$

The second last inequality shows that $d_{\Gamma'}(u) > d_{\Gamma}(v)$ and the last inequality is followed by $\sum_{i=1}^k d_{\Gamma}(u_i) \geq \sum_{i=h+1}^l d_{\Gamma}(v_i)$ and $d_{\Gamma}(u) \geq d_{\Gamma}(v)$. Hence, $SK_1(\Gamma') > SK_1(\Gamma)$. Which completes the proof. $\square$

Lemma 2.2 : Let Γ be a graph such that $\Gamma \in C_n^k$ and $n > k + 2$ then it is not a tree when $SK(\Gamma)$, $SK_1(\Gamma)$, $F(\Gamma)$ and $SK_2(\Gamma)$ are as large as possible.

Proof : On contrary suppose that Γ is a tree and $SK(\Gamma)$, $SK_1(\Gamma)$, $F(\Gamma)$ and $SK_2(\Gamma)$ are as large as possible. Let u_1 and u_2 are two non pendent and non adjacent vertices in Γ . Now there exist a new graph Γ' such that $\Gamma' = \Gamma \cup \{u_1 u_2\}$, which shows that $d_{\Gamma'}(u_1) = d_{\Gamma}(u_1) + 1$ and $d_{\Gamma'}(u_2) = d_{\Gamma}(u_2) + 1$, results Γ' is a cyclic graph such that

$$\begin{aligned} SK(\Gamma') &= SK(\Gamma) + \frac{1}{2} (d_{\Gamma'}(u_1)^2 + d_{\Gamma'}(u_2)^2 - d_{\Gamma}(u_1)^2 - d_{\Gamma}(u_2)^2) \\ &= SK(\Gamma) + \frac{1}{2} ((d_{\Gamma}(u_1) + 1)^2 + (d_{\Gamma}(u_2) + 1)^2 - d_{\Gamma}(u_1)^2 - d_{\Gamma}(u_2)^2) \end{aligned}$$

$$= SK(\Gamma) + \frac{1}{2}(d_r(u_1) + d_r(u_2) + 1)$$

Now the result is given as $SK(\Gamma') - SK(\Gamma) > 0$

One can see that $SK(\Gamma') > SK(\Gamma)$ and by lemma 2.1 $SK_1(\Gamma') > SK_1(\Gamma)$.

Now by using the definition of $F(\Gamma)$

$$F(\Gamma') = F(\Gamma) - d_r(u_1)d_r(u_1)^2 - d_r(u_2)d_r(u_2)^2 + d_r'(u_1)$$

$$d_r'(u_1)^2 + d_r'(u_2)d_r'(u_2)^2$$

By putting the values of $d_r'(u_1)$ and $d_r'(u_2)$, we can see that

$$F(\Gamma') = F(\Gamma) - d_r(u_1)d_r(u_1)^2 - d_r(u_2)d_r(u_2)^2 + (d_r(u_1) + 1)(d_r(u_1) + 1)^2 \\ + (d_r(u_2) + 1)(d_r(u_2) + 1)^2$$

$$F(\Gamma') = F(\Gamma) + 3d_r(u_1)d_r'(u_1) + 3d_r(u_2)d_r'(u_2) + 3$$

From above result, one can write it as, $F(\Gamma') - F(\Gamma) > 0$

Now, it is clear that $F(\Gamma) < F(\Gamma')$.

By using the definition of $SK_2(\Gamma)$, we have

$$SK_2(\Gamma') = SK_2(\Gamma) + \frac{1}{4}(F(\Gamma') - F(\Gamma)) + (SK_1(\Gamma') - SK_1(\Gamma))$$

As we know that $F(\Gamma') - F(\Gamma) > 0$ and $SK_1(\Gamma') - SK_1(\Gamma) > 0$ therefore $SK_2(\Gamma') - SK_2(\Gamma) > 0$, which implies that $SK_2(\Gamma') > SK_2(\Gamma)$. So, there is a contradiction to the choice of graph Γ . Hence, lemma is proved. $\square$

Lemma 2.3 : If $n \in \{k+1, k+2\}$ and $k > 1$ then $\Gamma \in C_n^k$ is a tree.

Lemma 2.4. If $SK(\Gamma)$, $SK_1(\Gamma)$, $F(\Gamma)$ and $SK_2(\Gamma)$ of a graph $\Gamma \in C_n^k$ attains the maximum value then all cycles are of length three except for at most one of the cycles of length four.

Proof : Contrarily, let C_n be the cycle in graph $\Gamma \in C_n^k$ say $C_n = c_1c_2c_3 \dots c_nc_1$ and $n \geq 5$, then there is a graph such that $\Gamma^* = (\Gamma - \{c_3c_4\}) \cup \{c_1c_3, c_1c_4\}$. and by using the definition of SK index and $d_{\Gamma^*}(c_1)$,

$$SK(\Gamma^*) = SK(\Gamma) + \frac{1}{2}((d_r(c_1) + 2)^2) - \frac{1}{2}(d_r(c_1)^2) \\ = SK(\Gamma) + \frac{1}{2}((d_r(c_1) + 2)^2 - d_r(c_1)^2) \\ = SK(\Gamma) + \frac{1}{2}((d_r(c_1)^2 + 4d_r(c_1) + 4 - d_r(c_1)^2)) \\ = SK(\Gamma) + 4(1 + d_r(c_1)) = SK(\Gamma) + 4 + 4d_r(c_1)$$

which shows that, $SK(\Gamma^*) - SK(\Gamma) > 0$.

Thus the result is $SK(\Gamma^*) > SK(\Gamma)$ and by lemma 2.1, $SK_1(\Gamma) < SK_1(\Gamma^*)$, which creates contradiction to the choice of graph. By using the definition of forgotten index $F(\Gamma)$

$$\begin{aligned} F(\Gamma^*) &= F(\Gamma) - d_{\Gamma}(c_1)^2 + d_{\Gamma^*}(c_1)^2 = F(\Gamma) - d_{\Gamma}(c_1)^2 + (d_{\Gamma}(c_1) + 2)^2 \\ &= F(\Gamma) - d_{\Gamma}(c_1)^2 + d_{\Gamma}(c_1)^2 + 4 + 4 \\ \Gamma(c_1) &= F(\Gamma) + 4(1 + \Gamma(c_1)) \end{aligned}$$

We can see that the difference is greater than zero, given as,

$$F(\Gamma^*) - F(\Gamma) > 0$$

Which results $F(\Gamma^*) > F(\Gamma)$. By using the definition of $SK_2(\Gamma)$, we can write that $SK_2(\Gamma^*) > SK_2(\Gamma)$ because $F(\Gamma^*) > F(\Gamma)$ and $SK_1(\Gamma) < SK_1(\Gamma^*)$. By proceeding this process, one can easily see that all cycles are of length three or four.

Let suppose there are two cycles having length four say, $C_1 = a_1a_2a_3a_4a_1$ and $C_2 = b_1b_2b_3b_4b_1$ in graph Γ . Since we have a cactus graph so, there will be a vertex say a_4 in C_1 such that there is no path that connects a_4 and b_1, a_4 and b_2 . Now there will be a new graph Γ^{**} such that $\Gamma^{**} = (\Gamma - a_1a_4, a_3a_4, b_1b_4) \cup \{a_1a_3, a_4b_1, a_4b_2, b_2b_4\}$

Since Γ^{**} has k pendent vertices, implies that $\Gamma^{**} \in C_n^k$. Now, by using lemma 2.1 and definitions of $SK(\Gamma)$, $SK_1(\Gamma)$, $F(\Gamma)$ and $SK_2(\Gamma)$ and $d\Gamma^{***}(b_2) = d_{\Gamma}(b_2) + 2$ one can easily find out that $SK(\Gamma^{**}) > SK(\Gamma)$, $SK_1(\Gamma^{**}) > SK_1(\Gamma)$, $F(\Gamma^{**}) > F(\Gamma)$ and $SK_2(\Gamma^{**}) > SK_2(\Gamma)$. Hence there is a contradiction to the choice of graphs. $\square$

Lemma 2.5. *Length of every dense path is one or except for at most one of them is two when a graph Γ has maximum $SK(\Gamma)$, $SK_1(\Gamma)$, $F(\Gamma)$ and $SK_2(\Gamma)$.*

Proof : On the contrary, Let $P = \rho_1\rho_2\rho_3 \dots \rho_{p-1}\rho_p i$ be the dense path and C be the cycle in the graph Γ such that $V(P) \cap V(C) = \{\rho_1\}$ and $d_{\rho} pi = 1$. If $p \geq 4$ then there is a graph $\Gamma^* = \Gamma \cup \{\rho_1\rho_{p-1}\}$ then $\Gamma^* \in \Gamma[n, k]$ and $d_{\Gamma^*}(\rho_1) = d_{\Gamma}(\rho_1) + 1$ and $d_{\Gamma^*}(\rho_{p-1}) = d_{\Gamma}(\rho_{p-1}) + 1$, we can see that

$$\begin{aligned} SK(\Gamma^*) &= SK(\Gamma) + \frac{1}{2}(d_{\Gamma^*}(\rho_{p-1})^2 + d_{\Gamma^*}(\rho_1)^2 - d_{\Gamma}(\rho_{p-1})^2 - d_{\Gamma}(\rho_1)^2) \\ SK(\Gamma^*) &= SK(\Gamma) + \frac{1}{2}(d_{\Gamma}(\rho_{p-1}) + d_{\Gamma}(\rho_1) + 1) \end{aligned}$$

$$SK(\Gamma^*) - SK(\Gamma) > 0$$

So, $SK(\Gamma^*) > SK$ and by lemma 2.1 $SK_1(\Gamma^*) > SK_1$. For $F(\Gamma)$, we can see that

$$F(\Gamma^*) = F(\Gamma) - d_{\Gamma}(\rho_{p-1})^3 - d_{\Gamma}(\rho_1)^3 + d_{\Gamma^*}(\rho_{p-1})^3 + d_{\Gamma^*}(\rho_1)^3$$

Which shows that $F(\Gamma^*) - F(\Gamma) > 0$ or $F(\Gamma^*) > F(\Gamma)$. Now by the definition of $SK_2(\Gamma)$, one can easily find that $SK_2(\Gamma^*) > SK_2(\Gamma)$ which is the contradiction to the choice of Γ . We can repeat this process until dense path are of length one or two.

Let suppose P_1 and P_2 are two paths of length two, say $P_1 = \rho_1' \rho_2' \rho_3' j$ and $P_2 = \rho^* 1 \rho^* 2 \rho^* 3'$ and C_1 and C_2 are two cycles such that $V(P_1) \cap V(C_1) = \{\rho^j 1\}$ and $V(P_2) \cap V(C_2) = \{\rho 1^*\}$ and $j, j' \geq 1$ then there is a new graph Γ^{**} such that $\Gamma^{**} = (G - \{\rho j 1 \rho j 2, \rho 2 j \rho 3 j 1\}) \cup \{\rho^j 1 \rho^j 3 1, \rho^* 1 \rho_2', \rho_2^* \rho^j 2\}$

Then $\Gamma^{**} \in \Gamma[n, k]$ and $d_{\Gamma^{**}}(\rho^j 2) = d_{\Gamma}(\rho^j 2) + 1$ and $d_{\Gamma^{**}}(\rho 1') = d_{\Gamma}(\rho 1') + 1$, which is contradiction to the choice of Γ because $SK(\Gamma^{**}) > SK(\Gamma)$, $SK_1(\Gamma^{**}) > SK_1(\Gamma)$, $F(\Gamma^{**}) > F(\Gamma)$ and $SK_2(\Gamma^{**}) > SK_2(\Gamma)$. Hence proved. $\square$

Lemma 2.6: If $SK(\Gamma)$, $SK_1(\Gamma)$, $F(\Gamma)$ and $SK_2(\Gamma)$ of a graph Γ are maximum then Γ has a dense path of length two or a cycle of length four but not both.

Proof: Let C_1 be the cycle and $P = \rho_1 \rho_2 \rho_{3i}$ be the path such that $V(C_1) \cap V(P) = \{\rho_1\}$ and $d_{\rho} 3i$ for $i \geq 1$. Now consider another cycle C_2 say $C_2 = b_1 b_2 b_3 b_4 b_1$. By using the definition of cactus graph there exist $b_i \in V(C_2)$ (say b_2) such that there is no path connecting b_2 and ρ_1 , b_2 and ρ_2 . Now there is a graph Γ^* such that $\Gamma^* = (\Gamma - \{b_1 b_2, b_2 b_3\}) \cup \{\rho_1 b_2, \rho_2 b_2, b_2 b_3\}$. Which results

$$\begin{aligned} SK(\Gamma^*) &= SK(\Gamma) + \frac{1}{2} (d_{\Gamma^*}(\rho_1)^2 + d_{\Gamma^*}(\rho_2)^2 - d_{\Gamma}(\rho_1)^2 - d_{\Gamma}(\rho_2)^2) \\ &= SK(\Gamma) + \frac{1}{2} ((d_{\Gamma}(\rho_1) + 1)^2 + (d_{\Gamma}(\rho_2) + 1)^2 - d_{\Gamma}(\rho_1)^2 - d_{\Gamma}(\rho_2)^2) \\ &= SK(\Gamma) + \frac{1}{2} (d_{\Gamma}(\rho_1) + d_{\Gamma}(\rho_2) + 1) \end{aligned}$$

From above equation one can easily see that,

$$SK(\Gamma^*) - SK(\Gamma) > 0$$

It implies that $SK(\Gamma^*) > SK(\Gamma)$ and by lemma 2.1 $SK_1(\Gamma^*) > SK_1(\Gamma)$. Now by the definition of $F(\Gamma)$,

$$F(\Gamma^*) = F(\Gamma) - d_{\Gamma}(\rho_1)^3 - d_{\Gamma}(\rho_2)^3 + d_{\Gamma^*}(\rho_1)^3 + d_{\Gamma^*}(\rho_2)^3$$

So, $F(\Gamma^*) > F(\Gamma)$. Now $SK_2(\Gamma^*) > SK_2(\Gamma)$ because $SK_1(\Gamma^*) - SK_1(\Gamma) > 0$ and $F(\Gamma^*) - F(\Gamma) > 0$ and Which is a contradiction.

Now, consider a cycle $C_3 = c_1 c_2 c_3 c_4 c_1$ of length four and dense path $P = \rho_1' \rho_2' \rho_3' 3 1$ of length two such that $V(C_3) \cap V(P) = c_i$ (say c_2), so dense path is $P = c_2 \rho_2' 2 \rho_3' 3 1$. Now there exist a new graph Γ'' such that $\Gamma'' = \Gamma - \{c_1 c_2, c_1 c_4\} \cup \{c_2 c_4, c_1 c_2, c_2 \rho_2' 2\}$

It is showing that $d_{\Gamma'}(c_2) = d_{\Gamma}(c_2) + 2$ and $d_{\Gamma'}(\rho_2) = d_{\Gamma}(\rho_2) + 1$ which creates a contra-diction to the choice of Γ because by using the definitions of $SK(\Gamma)$, $SK_1(\Gamma)$, $SK_2(\Gamma)$, $F(\Gamma)$ the results are $SK(\Gamma^{**}) > SK(\Gamma)$, $SK_1(\Gamma^{**}) > SK_1(\Gamma)$, $F(\Gamma^{**}) > F(\Gamma)$ and $SK_2(\Gamma^{**}) > SK_2(\Gamma)$. These are showing contradiction to the choice of graph. So, lemma is true. $\square$

Lemma 2.7. *Let C be the cycle in graph $\Gamma \in C_n^k$ and d_a, d_b are the degrees of the vertices a, b of the cycle C . If $\min\{d_a, d_b\} \geq 3$ then there exist a graph Γ' such that $SK(\Gamma') > SK(\Gamma)$, $SK_1(\Gamma') > SK_1(\Gamma)$, $F(\Gamma') > F(\Gamma)$ and $SK_2(\Gamma') > SK_2(\Gamma)$.*

Proof : Given C be the cycle in the graph Γ and $\min\{d_a, d_b\} \geq 3$, without loss of generality, let $d_a \geq d_b \geq 3$, then there exist a vertex w such that $w \in E(N(b) - V(C) - N(a))$. Now, there is a graph Γ' such that $\Gamma' = (\Gamma - \{wb\}) \cup \{wa\}$

One can see that $d_a \geq d_b \geq d_b - 1$, therefor

$$\begin{aligned} SK(\Gamma') &= SK(\Gamma) + \frac{1}{2}(d_{\Gamma'}(a)^2 + d_{\Gamma'}(b)^2 - d_{\Gamma}(a)^2 - d_{\Gamma}(b)^2) \\ &= SK(\Gamma) + \frac{1}{2}((d_{\Gamma}(a) + 1)^2 + (d_{\Gamma}(b) - 1)^2 - d_{\Gamma}(a)^2 - d_{\Gamma}(b)^2) \\ &= SK(\Gamma) + \frac{1}{2}(d_{\Gamma}(a) - d_{\Gamma}(b) + 1) \end{aligned}$$

Above equation shows that $SK(\Gamma') - SK(\Gamma) > 0$

Thus $SK(\Gamma') > SK(\Gamma)$ and lemma 2.1 shows that $SK_1(\Gamma) < SK_1(\Gamma')$. By the definition of $F(\Gamma)$, $F(\Gamma') = F(\Gamma) - d_{\Gamma}(a)^3 - d_{\Gamma}(b)^3 + (d_{\Gamma}(a) + 1)^3 + (d_{\Gamma}(b) - 1)^3$

By an elementary calculation, we have $F(\Gamma') - F(\Gamma) > 0$. Thus, $F(\Gamma') > F(\Gamma)$. Now we have $F(\Gamma') > F(\Gamma)$ and $SK_1(\Gamma) < SK_1(\Gamma')$ then by the definition of $SK_2(\Gamma') > SK_2(\Gamma)$. By the method of contradiction the lemma is true. $\square$

Lemma 2.8 : *$SK(\Gamma)$, $SK_1(\Gamma)$, $F(\Gamma)$ and $SK_2(\Gamma)$ are as large as possible then there will be a common vertex between any three cycles.*

Proof : In cactus graph, any two cycles do not have common edge. Let suppose that we have two disjoint cycles C_1, C_2 and they are connected by path $P = \rho_1 \rho_2 \rho_3 \dots \rho_p$ and it is as short as possible such that $V(P) \cap V(C_1) = \{\rho_1\}$ and $V(P) \cap V(C_2) = \{\rho_p\}$.

Consider that the path has no common edge with any other cycle in Γ and $|V(P)| \geq 3$. Let the new graph $\Gamma' = \Gamma \cup \{\rho_1 \rho_p\}$ and $\Gamma' \in \Gamma(n, k)$, one can see that $d_{\Gamma'}(\rho_1) = d_{\Gamma}(\rho_1) + 1$ and $d_{\Gamma'}(\rho_p) = d_{\Gamma}(\rho_p) + 1$. By using the definitions of $SK(\Gamma)$, $SK_1(\Gamma)$, $SK_2(\Gamma)$ and $F(\Gamma)$ and lemma 2.1 we can easily calculate that $SK(\Gamma') > SK(\Gamma)$, $SK_1(\Gamma') > SK_1(\Gamma)$, $F(\Gamma') > F(\Gamma)$ and $SK_2(\Gamma') > SK_2(\Gamma)$. If $|V(P)| = 2$, without loss of generality $d_{\Gamma}(\rho_1) \geq d_{\Gamma}(\rho_2)$ and $C_2 =$

$c_1c_2c_3...c_1$ be the cycle. As $V(C_2) \cap V(P) = \{\rho_2\}$ then $C_2 = \rho_2c_2c_3...c_2$ and we have $c_2 \in N(\rho_1)$. If $c_2 \in N(\rho_1)$ then it does not hold the definition of cactus graph. Let $\Gamma^* = (\Gamma - \{\rho_2c_2\}) \cup \{\rho_1c_2\}$ which implies that $SK(\Gamma^*) - SK(\Gamma) > 0$, $SK_1(\Gamma^*) - SK_1(\Gamma) > 0$, $F(\Gamma^*) - F(\Gamma) > 0$, $SK_2(\Gamma^*) - SK_2(\Gamma) > 0$. which is the contradiction to the choice of Γ . So, $F(\Gamma^*) > F(\Gamma)$, $SK_1(\Gamma) < SK_1(\Gamma^*)$ and $SK_2(\Gamma) < SK_2(\Gamma^*)$. If P has some common edge with another cycle, say C_3 , by the choice of C_1 and C_2 and the definition of cactus graph, we have $C_1 \cap C_3 = \{\rho_1\}$ and $C_2 \cap C_3 = \{\rho_p\}$. By lemma 2.7, there will be a new graph Γ'' such that $F(\Gamma'') > F(\Gamma)$, $SK_1(\Gamma) < SK_1(\Gamma'')$ and $SK_2(\Gamma) < SK_2(\Gamma'')$. So, lemma is true. $\square$

Lemma 2.9 : If $SK(\Gamma)$, $SK_1(\Gamma)$, $F(\Gamma)$ and $SK_2(\Gamma)$ attains maximum value and a tree T is attached to a vertex u_0 of a cycle of graph Γ , then $d_u \leq 2$ for any $u \in V(T) - \{u_0\}$.

Proof : Let Γ be a graph with maximum $M_i(\Gamma)$, $i \in 1, 2$. On contrary assume that a vertex $u \in V(T) - u_0$ has degree $d_u \geq 3$ and closest to the pendent vertex. $Ford(u, u_0) \geq 2$, we have $\Gamma^* = \Gamma \cup \{u_0u\}$, $\Gamma^* \in \Gamma[n, k]$, which shows that,

$$\begin{aligned} SK(\Gamma^*) &= SK(\Gamma) + \frac{1}{2}(d_{\Gamma^*}(u_0)^2 + d_{\Gamma^*}(u)^2 - d_{\Gamma}(u_0)^2 - d_{\Gamma}(u)^2) \\ &= SK(\Gamma) + \frac{1}{2}((d_{\Gamma}(u_0) + 1)^2 + (d_{\Gamma}(u) + 1)^2 - d_{\Gamma}(u_0)^2 - d_{\Gamma}(u)^2) \\ &= SK(\Gamma) + \frac{1}{2}(d_{\Gamma}(u_0) + d_{\Gamma}(u) + 1) \end{aligned}$$

Thus, the result is $SK(\Gamma^*) - SK(\Gamma) > 0$. And $F(\Gamma^*) = F(\Gamma) - d_{\Gamma}(u_0)d_{\Gamma}(u_0)^2 - d_{\Gamma}(u)d_{\Gamma}(u)^2 + d_{\Gamma^*}(u)d_{\Gamma^*}(u)^2 + d_{\Gamma^*}(u_0)d_{\Gamma^*}(u_0)^2$

By putting the values of $d_{\Gamma^*}(u_0)$ and $d_{\Gamma^*}(u)$, we can see that

$$F(\Gamma^*) = F(\Gamma) + 3d_{\Gamma}(u_0)d_{\Gamma^*}(u_0) + 3d_{\Gamma}(u)d_{\Gamma^*}(u) + 3F(\Gamma^*) - F(\Gamma) > 0$$

So, $SK(\Gamma^*) > SK(\Gamma)$ and $F(\Gamma^*) > F(\Gamma)$. By lemma 2.1 $SK_1(\Gamma^*) > SK_1(\Gamma)$ and by using the definition of $SK_2(\Gamma)$, $SK_2(\Gamma^*) > SK_2(\Gamma)$. Hence, contradiction to the choice of graph. For $d(u, u_0) = 1$ let $\{v_1v_2v_3...v_{d_u-2}\}$ be the $d_u - 2$ neighbors of u such that $d(v_i, u_0) > d(u, u_0)$, v be a neighbor of u_0 which belongs to a cycle C_0 .

By lemma 2.6 all cycles are of length 3. Consider u_0uv_1 be a pendent path and $C_0 = u_0v_1vu_0$ be a cycle, $\Gamma' = (\Gamma - uv_1) \cup \{u_0v_1\}$ and $\Gamma'' = (\Gamma - u_0v) \cup \{uv\}$, then $\Gamma', \Gamma'' \in \Gamma[n, k]$, which shows that $d_{\Gamma'}(u) = d_u - 1$, $d_{\Gamma'}(u_0) = du_0 + 1$ and $d_{\Gamma''}(u) = d_u + 1$, $d_{\Gamma''}(u_0) = du_0 - 1$. By lemma 2.1 $SK_1(\Gamma') > SK_1(\Gamma)$ and

$SK_1(\Gamma'') > SK_1(\Gamma)$. Now, by using the definition of $SK(\Gamma)$, if $du_0 \geq d_u$ then we have

$$\begin{aligned} SK(\Gamma') &= SK(\Gamma) + \frac{1}{2} ((d_r(u_0) + 1)^2 + (d_r(u) - 1)^2 - d_r(u_0)^2 - d_r(u)^2) SK(\Gamma') \\ &= SK(\Gamma) + \frac{1}{2} (d_r(u_0) - d_r(u) + 1) SK(\Gamma') - SK(\Gamma) > 0 \end{aligned}$$

and if $d_u > d_{u_0}$ then we have

$$\begin{aligned} SK(\Gamma'') &= SK(\Gamma) + \frac{1}{2} ((d_r(u) + 1)^2 + (d_r(u_0) - 1)^2 - d_r(u_0)^2 - d_r(u)^2) SK(\Gamma'') \\ &= SK(\Gamma) + \frac{1}{2} (d_r(u) - d_r(u_0) + 1) SK(\Gamma'') - SK(\Gamma) > 0 \end{aligned}$$

Thus $SK(\Gamma') > SK(\Gamma)$ and $SK(\Gamma'') > SK(\Gamma)$. By lemma 2.1 shows that $SK_1(\Gamma) < SK_1(\Gamma'')$ and $SK_1(\Gamma) < SK_1(\Gamma')$. Now By the elementary calculation using the definition of $F(\Gamma)$, one can easily find out that $F(\Gamma') > F(\Gamma)$ and $F(\Gamma'') > F(\Gamma)$. Now by the definition of $SK_2(\Gamma)$ we can easily find out that $SK_2(\Gamma') > SK_2(\Gamma)$ and $SK_2(\Gamma'') > SK_2(\Gamma)$. By the method of contradiction the lemma is true. $\square$

Lemma 2.10 : Let Γ be a graph with maximum $SK(\Gamma)$, $SK_1(\Gamma)$, $F(\Gamma)$ and $SK_2(\Gamma)$ then all trees in graph Γ are attached to a common vertex.

Proof : On contrary, assume that the trees T_1 and T_2 are attached with cycle C_1 and C_2 such that $V(C_1) \cap V(T_1) = \{v\}$ and $V(C_2) \cap V(T_2) = \{v'\}$ respectively. By lemma 2.8, all cycles in graph $\Gamma \in C_n^k$ have only one common vertex, say u , without loss of generality $v \neq v'$. Now, we have $d_v, dv_1, d_u \geq 3$. By using lemma 2.7 and 2.1 there exist a new graph Γ^* such that $M_1(\Gamma^*) > M_1(\Gamma)$, similarly $M_2(\Gamma^*) > M_2(\Gamma)$. And also by using the definitions of $SK(\Gamma)$ indices, $SK(\Gamma^*) > SK(\Gamma)$, $SK_1(\Gamma^*) > SK_1(\Gamma)$ and $F(\Gamma^*) > F(\Gamma)$. By the definition of SK_2 , $SK_2(\Gamma^*) > SK_2(\Gamma)$. Which is a contradiction to the choice of graph. $\square$

Lemma 2.11 : If a graph $\Gamma \in C_n^k$ having pendent vertices $k > 0$ and atmost one cycle of length four then there exist a graph Γ' such that $SK_1(\Gamma') > SK_1(\Gamma)$ and $SK_2(\Gamma') > SK_2(\Gamma)$.

Proof : If a graph has pendent vertices $k = 0$ then graph must have cycles of length three or four. Now consider a graph having pendent vertices $k > 0$ and atmost one cycle C of length four $C = c_0c_1c_2c_3$ attached with vertex u_0 of Γ such that $u_0 = c_0$ and $d_{u_0} > 2$. Let v_0 be a pendent vertex then there is a graph Γ' such that $\Gamma' = (\Gamma - \{c_1c_2, c_2c_3\}) \cup \{c_1c_3, v_0c_2\}$ then, we know that $M_2(\Gamma') - M_2(\Gamma) = d_{u_0} - 2$ then after multiplication on both side by $\frac{1}{2}$,

result is $\frac{1}{2}(M_2(\Gamma') - M_2(\Gamma)) = \frac{1}{2}(d_{u_0} - 2)SK_1(\Gamma') - SK_1(\Gamma) = \frac{1}{2}d_{u_0} - 1$ and similarly,

$$SK_2(\Gamma') - SK_2(\Gamma) = \frac{1}{4}(F(\Gamma') - F(\Gamma)) + (SK_1(\Gamma') - SK_1(\Gamma))$$

By putting the value of $SK_1(\Gamma') - SK_1(\Gamma)$ and $F(\Gamma') - F(\Gamma) = 0$ then, $SK_1(\Gamma') - SK_1(\Gamma) = \frac{1}{2}d_{u_0} - 1$. Here one can see that $SK_1(\Gamma') > SK_1(\Gamma)$ and $SK_2(\Gamma') > SK_2(\Gamma)$. Hence lemma is true. $\square$

We shall prove our theorems by using the conditions discussed in lemmas. By lemma 2.2, if $n \in k + 2$ then the graph $\Gamma \in C_n^k$ is not a tree; Lemma 2.3 shows that if $n \in \{k + 1, k + 2\}$, $k > 0$ then graph is a tree. If $SK(\Gamma)$, $F(\Gamma)$, $SK_1(\Gamma)$ and $SK_2(\Gamma)$ have maximum values then by lemma 2.4 and 2.5 all cycles are of length three except atmost one of them is four and the length dense path is one except atmost one of them is two; lemma 2.6 shows that in a graph, if possible, there exists a cycle of length four or a dense path of length two but not both; By lemma 2.7 and 2.9 all trees attached to a vertex u_0 of a cycle of graph Γ then $d_u \leq 2$ for any $u \in V(T) - u_0$; By lemma 2.10, all trees are attached to a common vertex of a cycle. If d_a and d_b are the degrees of any two vertices a, b of cycle C in graph Γ and $\min\{d_a, d_b\} \geq 3$ then there exist a graph Γ' such that $SK(\Gamma')$, $F(\Gamma')$, $SK_1(\Gamma')$ and $SK_2(\Gamma')$ have maximum values. Lemma 2.11 shows that If a graph $\Gamma \in C_n^k$ having pendent vertices $k > 0$ and atmost one cycle of length four then there exist a graph Γ' such that $SK_1(\Gamma') > SK_1(\Gamma)$ and $SK_2(\Gamma') > SK_2(\Gamma)$. By using the lemmas given above, we have following four graphs with the name $\zeta^1(n, k)$, $\zeta^2(n, k)$, $\zeta^3(n, k)$ and $\zeta^4(n, k)$, which can give us maximum values of $SK(\Gamma)$, $F(\Gamma)$, $SK_1(\Gamma)$ and $SK_2(\Gamma)$ indices.

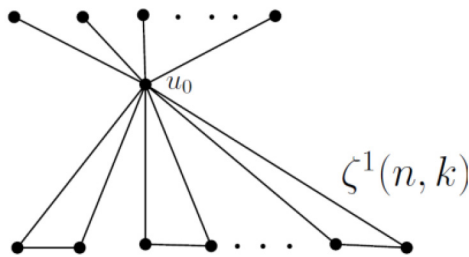


Figure 1

$\zeta^1(n, k)$ only has k pendant paths of length one and $\frac{n-k-1}{2}$ cycles of length three, where $n - k \equiv 1 \pmod{2}$.

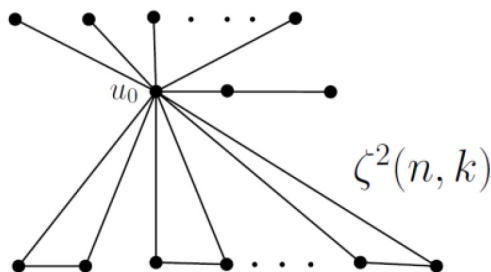


Figure 2

$\zeta^2(n, k)$ only has $k - 1$ pendant paths of length one, one of length two and $\frac{n-(k+2)}{2}$ cycles of length three, where $n - k \equiv 0 \pmod{2}$.

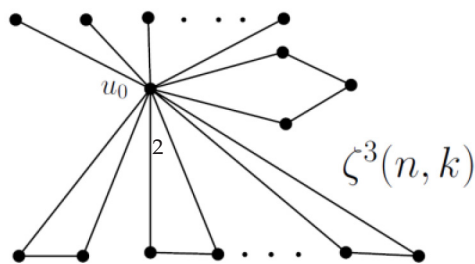


Figure 3

$\zeta^3(n, k)$ only has k pendant paths of length one, one cycle of length four and $\frac{n-(k+4)}{2}$ cycles of length three, where $n - k \equiv 0 \pmod{2}$.

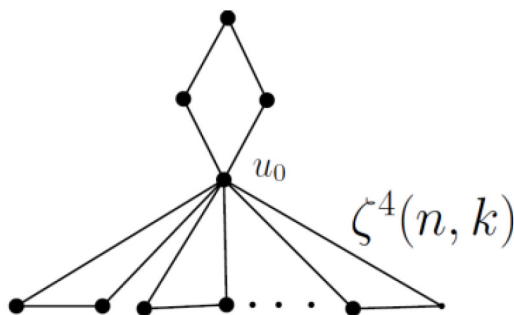


Figure 4

$\zeta^4(n, k)$ only has one cycle of length four and $\frac{n-4}{2}$ cycles of length three such that $k = 0$, where $n - k \equiv 0 \pmod{2}$.

2. Sharp Upper Bound of Cactus Graph for $SK(\Gamma)$

Sharp upper bound of cactus graphs using $SK(\Gamma)$ is given by the following theorem.

Theorem 3.1 : Let C_n^k be the family of cactus graphs with n vertices and k pendent vertices such that $k \geq 0$. Suppose the graph $\Gamma \in C_n^k$ then $SK(\Gamma)$ is

$$(SK(\Gamma)) \leq \begin{cases} \frac{n(n+2) - 3(k+1)}{2} & \text{if } n - k \equiv 1 \pmod{2} \\ \frac{n^2 - 3k}{2} & \text{if } n - k \equiv 0 \pmod{2} \end{cases}$$

Equality holds if and only if $\Gamma \approx \zeta^1(n, k)$ and $\Gamma \approx \zeta^2(n, k)$ or, $\zeta^3(n, k)$ respectively. $\zeta^1(n, k)$, $\zeta^2(n, k)$ and $\zeta^3(n, k)$ are shown in Figs. 1, 2 and 3 respectively.

Proof : By using following lemmas 1, 4-10 and lemma, we can see that the graphs $\Gamma \in C_n^k$ which give us maximum $SK(\Gamma)$ are $\zeta^1(n, k)$, $\zeta^2(n, k)$ and $\zeta^3(n, k)$. So, when $n - k \equiv 1 \pmod{2}$

$$\begin{aligned} SK(\Gamma) &\leq \frac{1}{2}((n - k - 1)(2 + (n - 1)) + k((n - 1) + 1) + (2 + 2)\left(\frac{n - k - 1}{2}\right)) \\ &= \frac{(1 + n)(n - k - 1) + n(k) + 2(n - k - 1)}{2} = \frac{n(n + 2) - 3(k + 1)}{2} \end{aligned}$$

So,

$$\begin{aligned} SK(\Gamma) &\leq \frac{1}{2}((n - k - 1)(2 + (n - 2)) + (k - 1)((n - 2) + 1) \\ &\quad + (2 + 2)\left(\frac{n - k - 2}{2}\right) + (2 + 1)) \\ &= \frac{1}{2}(n^2 - k(n) - n + k(n) - n - k + 1 + 3 + 2n - 2k - 2) = \frac{n^2 - 3k}{2} \end{aligned}$$

So, the result is $SK(\Gamma) \leq \frac{n^2 - 3k}{2}$. Hence the theorem is proved. $\square$

3. Sharp Upper Bound of Cactus Graph for $SK_1(\Gamma)$

Sharp upper bound of cactus graphs using $SK_1(\Gamma)$ index is given by the following theorem.

Theorem 4.1 : Let C_n^k be the family of cactus graphs with n vertices and k pendent vertices. Suppose the graph $\Gamma \in C_n^k$ then $SK_1(\Gamma)$ is

$$SK_1(\Gamma) \leq \begin{cases} \frac{2n(n-1)-k(n+1)}{2} & \text{if } n-k \equiv 1 \pmod{2}, k \geq 0 \\ \frac{n(2n-k-5)+4}{2} & \text{if } n-k \equiv 0 \pmod{2}, k > 0 \\ n^2-3n+4 & \text{if } n-k \equiv 0 \pmod{2}, k = 0 \end{cases}$$

Equality holds if and only if $\Gamma \approx \zeta^1(n, k)$, $\Gamma \approx \zeta^2(n, k)$ and $\Gamma \approx \zeta^4(n, k)$ respectively.

$\zeta^1(n, k)$, $\zeta^2(n, k)$ and $\zeta^4(n, k)$ are given in Figs. 1, 2 and 4 respectively.

Proof : By using following lemmas 1-11 which shows that the graph may have a pendent path of length two but not cycle of length four when $k > 0$. So, we can see that the graphs $\Gamma \in C_n^k$ which give us maximum $SK_1(\Gamma)$ are $\zeta^1(n, k)$, $\zeta^2(n, k)$ and $\zeta^4(n, k)$. So, when $n-k \equiv 1 \pmod{2}$

$$\begin{aligned} SK_1(\Gamma) &\leq \frac{1}{2} \left(2(n-1)(n-k-1) + (n-1)(k)(1) + 2(2) \left(\frac{n-k-1}{2} \right) \right) \\ &= \frac{1}{2} \left((2n-2)(n-k-1) + k(n-1) + 4 \left(\frac{n-k-1}{2} \right) \right) \\ &= \frac{1}{2} (4n^2 - 2nk - 2n - 2n + 2k + 2 + nk + 2n - k - 2k - 1) \\ &= \frac{2n^2 - 2n - n(k) - k}{2} = \frac{2n(n-1) - k(n+1)}{2} \end{aligned}$$

Which results, $SK(\Gamma) \leq \frac{2n(n-1)-k(n+1)}{2}$. and when $n-k \equiv 0 \pmod{2}$, $k > 0$

$$\begin{aligned} SK_1(\Gamma) &\leq \frac{1}{2} \left(2(n-2)(n-k-1) + (n-2)(k-1)(1) + 2(2) \left(\frac{n-k-2}{2} \right) + 2 \right) \\ &= \frac{2n^2 - 5n - n(k) + 4}{2} = \frac{n(2n-k-5) + 4}{2} \end{aligned}$$

Thus, $SK(\Gamma) \leq \frac{n(2n-k-5)+4}{2}$. and when $n-k \equiv 0 \pmod{2}$, $k=0$, then

$$\begin{aligned} SK_1 &\leq \frac{1}{2} (2n^2 - 6n + 8) \\ SK_1 &\leq n^2 - 3n + 4 \end{aligned}$$

Hence the theorem is proved. $\square$

4. Sharp Upper Bound of Cactus Graph for $F(\Gamma)$

Sharp upper bound of cactus graphs using $F(\Gamma)$ index is given by the following theorem.

Theorem 5.1 : Let C_n^k be the family of cactus graphs with n vertices and k pendent vertices such that $k \geq 0$. Suppose the graph $\Gamma \in C_n^k$ then $F(\Gamma)$ is

$$F(\Gamma) \leq \begin{cases} n(n^2 - 3n + 11) - 7k - 9 & \text{if } n - k \equiv 1 \pmod{2} \\ n(n^2 - 6n + 20) - 7k - 16 & \text{if } n - k \equiv 0 \pmod{2} \end{cases}$$

Equality holds if and only if $\Gamma \approx \zeta^1(n, k)$ and $\Gamma \approx \zeta^2(n, k)$ or, $\zeta^3(n, k)$ respectively. $\zeta^1(n, k)$, $\zeta^2(n, k)$ and $\zeta^3(n, k)$ are shown in Figs. 1, 2 and 3 respectively.

Proof : By using following lemmas 1-10, we can see that the graphs $\Gamma \in C_n^k$ which give us maximum $F(\Gamma)$ are $\zeta^1(n, k)$, $\zeta^2(n, k)$ and $\zeta^3(n, k)$. So, when $n - k \equiv 1 \pmod{2}$, $k \geq 0$

$$F(\Gamma) \leq ((n-1)^2 + 2^2)(n-k-1) + (2^2 + 1) \left(\frac{n-k-1}{2} \right) + ((n-1)^2 + 1)(k)$$

$$= (n^2 - 2n + 5)(n-k-1) + 4(n-k-1) + k(n^2 - 2n + 2)$$

$$= n^3 - 3n^2 + 11n - 7k - 9 = n(n^2 - 3n + 11) - 7k - 9$$

so, $F(\Gamma) \leq n(n^2 - 3n + 11) - 7k - 9$ and when $n - k \equiv 0 \pmod{2}$

$$F(\Gamma) \leq ((n-1)^2 + 2^2)(n-k-1) + (2^2 + 2^2) \left(\frac{n-k-2}{2} \right)$$

$$+ ((n-2)^2 + 1)(k-1 + (2^2 + 1)) = n^3 - 6n^2 + 20n - 7k - 16$$

$$= n(n^2 - 6n + 20) - 7k - 16$$

Which results, $F(\Gamma) \leq n(n^2 - 6n + 20) - 7k - 16$. Hence the theorem is proved. $\square$

5. Sharp Upper Bound of Cactus Graph for $SK_2(\Gamma)$

Sharp upper bound of cactus graphs using $SK_2(\Gamma)$ index is given by the following theorem.

Theorem 6.1 : Let C_n^k be the family of cactus graphs with n vertices and k pendent vertices. Suppose the graph $\Gamma \in C_n^k$ then $SK_2(\Gamma)$ is

$$SK_2(\Gamma) \leq \begin{cases} \frac{n^2(n+1) - n(2k-7) - 9(k+1)}{4} & \text{if } n-k \equiv 1 \pmod{2}, k \geq 0 \\ \frac{n^2(n-2) + 2n(5-k) - 7k - 8}{4} & \text{if } n-k \equiv 0 \pmod{2}, k > 0 \\ \frac{n^2(n-2) + 8n}{4} & \text{if } n-k \equiv 0 \pmod{2}, k = 0 \end{cases}$$

Equality holds if and only if $\Gamma \approx \zeta^1(n, k)$, $\Gamma \approx \zeta^2(n, k)$ and $\Gamma \approx \zeta^4(n, k)$ respectively. $\zeta^1(n, k)$, $\zeta^2(n, k)$ and $\zeta^4(n, k)$ are given in Figs. 1, 2 and 4 respectively.

Proof : By using following lemmas 1-11 which shows that the graph may have a pendent path of length two but not cycle of length four when $k > 0$. So, we can see that the graphs $\Gamma \in C_n^k$ which give us maximum $SK_2(\Gamma)$ are $\zeta^1(n, k)$, $\zeta^2(n, k)$ and $\zeta^4(n, k)$. So, when $n-k \equiv 1 \pmod{2}$

$$\begin{aligned} SK_2(\Gamma) &= \frac{1}{4}F(\Gamma) + SK_1(\Gamma)SK_2(\Gamma) \leq \frac{1}{4}(n^3 - 3n^2 + 11n - 7k - 9) \\ &\quad + \frac{2n^2 - 2n - k(n) - k}{2} = \frac{n^3 + n^2 + 7n - 2k(n) - 9k - 9}{4}SK_2(\Gamma) \\ &\leq \frac{n^2(n+1) - n(2k-7) - 9(k+1)}{4} \end{aligned}$$

and when $n-k \equiv 0 \pmod{2}$, $k > 0$

$$\begin{aligned} SK_2(\Gamma) &\leq \frac{1}{4}(n^3 - 6n^2 + 20n - 7k - 16) + \frac{2n^2 - n(k) - 5n + 4}{2} \\ &= \frac{n^3 - 2n^2 + 10n - 2k(n) - 7k - 8}{4} = \frac{n^2(n-2) + 2n(5-k) - 7k - 8}{4} \end{aligned}$$

Which gives $SK_2(\Gamma) \leq \frac{n^2(n-2) + 2n(5-k) - 7k - 8}{4}$ and when $n-k \equiv 0 \pmod{2}$, $k = 0$

$$\begin{aligned} SK_2(\Gamma) &\leq \frac{1}{4}(n^3 - 6n^2 + 20n - 7k - 16) + \frac{n^2 - 3n + 4}{2} \\ SK_2(\Gamma) &\leq \frac{n^2(n-2) + 8n - 7k}{4} \end{aligned}$$

As $k = 0$, therefor $SK_2 \leq \frac{n^2(n-2) + 8n}{4}$ Hence the theorem is proved. $\square$

6. Conclusion

There are different Molecular descriptors that have been used successfully in many QSAR/QSPR studies. In this paper we determined the sharp upper bounds for $SK(\Gamma)$ and forgotten indices of cactus graphs. We also characterized the extremal graphs for these indices. It would be interesting to derive similar results for other famous indices.

Acknowledgments

The authors declare that they have no competing interests, and they equally contributed to the paper. This research is supported by UGC-SAP-DRS-11, No.F. 510/12/DRS-11/2018 (SAP-I), dated April 9, 2018.

References

- [1] Liu, J.B., Nadeem, M.F., Siddiqui, H.M.A., Nazir, W. (2019). Computing metric dimension of certain families of toeplitz graphs. *IEEE Access*, 7, 126734-126741. <https://doi.org/10.1109/ACCESS.2019.2938579>
- [2] Raheem, A., Hasni, R., Javaid, M., Umar, M. A. (2020). On cordial related labeling of isomorphic copies of paths and subdivision of star. *Journal of Discrete Mathematical Sciences and Cryptography*, 23(7), 1381-1390. <https://doi.org/10.1080/09720529.2019.1698802>
- [3] Siddiqui, H M.A., Hayat, S., Khan, A., Imran, M., Razzaq, A., Liu, J.B. (2019). Resolvability and fault-tolerant resolvability structures of convex polytopes. *Theoretical Computer Science*, 796, 114-128. <https://doi.org/10.1016/j.tcs.2019.08.032>
- [4] Zhang, F., Nazeer, S., Habib, M., Zia, T.J., Ren, Z. (2019). Radio Number for Generalized Petersen Graphs $P(n,2)$. *IEEE Access*, 7, 142000-142008. <https://doi.org/10.1109/ACCESS.2019.2943835>
- [5] Rafiullah, M., Siddiqui, H.M.A., Ahmad, S. (2019). Resolvability of some convex polytopes. *Utilitas Mathematica*, 111, 309-323.
- [6] Schenker, A., Mark L., Horst B., Abraham K. Clustering of web documents using a graph model. In *Web Document Analysis: Challenges and Opportunities*, 3-18. 2003.
- [7] Marx, D. (2004). Graph colouring problems and their applications in scheduling, *Periodica Polytechnica Electrical Engineering*, 48(1-2), 11-16.
- [8] Eswaramurthy, V.P. New algorithm for analyzing performance of neighborhood strategies in solving job shop scheduling problems. *Journal of Scientific Industrial Research*, (2008).

- [9] Wiener, H. (1947). Structural determination of paraffin boiling points. *Journal of the American chemical society*, 69(1), 17-20. <https://doi.org/10.1021/ja01193a005>
- [10] Shigehalli, V.S., Kanabur, R. (2016). Computation of new degree-based topological indices of graphene. *Journal of Mathematics*, 2016. <https://doi.org/10.1155/2016/4341919>
- [11] Gutman, I. (2011). Multiplicative Zagreb indices of trees. *Bull. Soc. Math. Banja Luka*, 18, 17-23.
- [12] Klavzar, S., Rajapakse, A., Gutman, I. (1996). The Szeged and the Wiener index of graphs. *Applied Mathematics Letters*, 9(5), 45-49.
- [13] Akhter, N., Jamil, M.K., Tomescu, I. (2016). Extremal first and second Zagreb indices of apex trees. *Jangjeon Mathematical Society*, 78(4)
- [14] Wang, S., Wei, B. (2016). Multiplicative Zagreb indices of cacti. *Discrete Mathematics, Algorithms and Applications*, 8(03), 1650040. <https://doi.org/10.1142/S1793830916500403>
- [15] Furtula, B., Gutman, I. (2015). A forgotten topological index. *Journal of Mathematical Chemistry*, 53(4), 1184-1190. <https://doi.org/10.1007/s10910-015-0480-z>
- [16] Martinez-Prez, J., Rodriguez, J. M. (2019). Some results on lower bounds for topological indices. *Journal of Mathematical Chemistry*, 57(5), 1472-1495.
- [17] Ghanbari, N., Alikhani, S. (2021). Sombor index of certain graphs. *arXiv preprint arXiv:2102.10409*.
- [18] Khadikar, P.V. (2000). On a novel structural descriptor PI. *National Academy Science Letters* 23(7-8), 113-118
- [19] Shigehalli, V.S., Kanabur, R. (2016). Computation of new degree-based topological indices of graphene. *Journal of Mathematics* 2016(1), 1-6 [10.1155/2016/4341919](https://doi.org/10.1155/2016/4341919)
- [20] Wang, H., Kang, L. (2015). On the Harary index of cacti. *Utilitas Mathematica*. 96, 149-163.
- [21] Ahmad, M. S., Nazeer, W., Kang, S. M., Imran, M., Gao, W. (2017). Calculating degree-based topological indices of dominating David derived networks. *Open Physics*, 15(1), 1015-1021. <https://doi.org/10.1515/phys-2017-0126>
- [22] Ahmad, M., Afzal, D., Nazeer, W., Kang, S. (2017). On topological indices of octagonal network. *Far East Journal of Mathematical Sciences*, 102, 2563-2571.

- [23] Ravi, V., Desikan, K. (2021). Neighbourhood Degree-Based Topological In-dices of Graphene Structure. *Biointerface Research in Applied Chemistry*, 11(5),13681-13694.
- [24] Alameri, A., Shubatah, M., Alsharafi, M. (2020). Zagreb indices, Hyper Zagreb indices and Redefined Zagreb indices of conical graph. *Advances in Mathematics: Scientific Journal*, 9(6), 3631-3642.
- [25] Lokesha, V., Yasmeen, K.Z., Manjunath, M., Venkatachalam, M. (2020). Lower and Upper bounds of SK indices of F-join of graphs. *International Journal of Open Problems in Computer Science Mathematics*, 13(4).
- [26] Lokesha, V., Yasmeen, K.Z. (2019). SK indices, forgotten topological indices and hyper Zagreb index of Q operator of carbon nanocone. *TWMS Journal of Applied and Engineering Mathematics*, 9(3), 675-680. <http://jaem.isikun.edu.tr/web/images/articles/vol.9.no.3/28.pdf>
- [27] Ranjini, P. S. W., Lokesha, V. (2020). SK Indices of Graph Operator $S(G)$ and $R(G)$ On Few Nanostructures. *Montes Taurus Journal of Pure and Applied Mathematics*, 2(2), 38-44.
- [28] Furtula, B., Gutman, I. (2015). A forgotten topological index. *Journal of mathematical chemistry*, 53(4), 1184-1190. <https://doi.org/10.1007/s10910-015-0480-z>
- [29] Gao, W., Siddiqui, M.K., Imran, M., Jamil, M.K., Farahani, M.R. (2016). Forgotten topological index of chemical structure in drugs. *Saudi Pharmaceutical Journal*, 24(3), 258-264. <https://doi.org/10.1016/j.jsps.2016.04.012>
- [30] Siddiqui, H., Farahani, M.R. (2017). Forgotten polynomial and forgotten in-dex of certain interconnection networks. *Open Journal of Mathematical Analysis*, 1(1), 44-59. <https://doi.org/10.30538/psrp-oma2017.0005>
- [31] Alsinai, A., Alwardi, A., Ahmed, H., Soner, N.D. (2021). Leap Zagreb indices for the Central graph of graph. *Journal of Prime Research in Mathematics*, 17(2), 73-78.
- [32] Alsinai, A., Ahmed, H., Alwardi, A., & Soner, N.D. (2021). HDR Degree Based Indices and Mhr-Polynomial for the Treatment of COVID-19, *Biointerface Research in Applied Chemistry*, 12,(6), 2022, 7214-7225. <https://doi.org/10.33263/BRIAC126.72147225>.
- [33] Alsinai, A., Basavanagoud, B., Sayyed, Farahani, M. R. (2021). Sombor index of some nanostructures, graph of graph. *Journal of Prime Research in Mathematics*, 17(2),123-133.
- [34] Alsinai, A., Alwardi, A., Soner, N.D. (2021). On Reciprocal leap function of graph. *Journal of Discrete Mathematical Sciences and*

Cryptography, 24(2), 307-324. <https://doi.org/10.1080/09720529.2021.1882154>

- [35] Alsinai, A., Alwardi, A., Soner, N.D. (2021). Topological Properties of Graphene Using Y_k polynomial. In *Proceedings of the Jangjeon Mathematical Society* (Vol. 24, No. 3).
- [36] Afzal, F., Alsinai, A., Hussain, S., Afzal, D., Chaudhry, F., Cancan, M. (2021). On topological aspects of silicate network using M -polynomial. *Journal of Discrete Mathematical Sciences and Cryptography*, 1-11. <https://doi.org/10.1080/09720529.2021.1977486>
- [37] Hasan, A., Qasmi, M.H.A., Alsinai, A., Alaeiyan, M., Farahani, M.R., Cancan, M. (2021). Distance and Degree Based Topological Polynomial and Indices of X -Level Wheel Graph. *Journal of Prime Research in Mathematics*, 17(2), 39-50.
- [38] Alsinai, A., Alwardi, A., Farahani, M. R., Soner, N.D. (2021). On the ψ_k -polynomial of graph. *Eurasian Chemical Communications*, 3(4), 219-226. <https://doi.org/10.22034/ecc.2021.274069.1138>
- [39] Alsinai, A., Alwardi, A., Soner, N.D. (2021). On Reciprocals Leap Indices of Graphs. *International Journal of Analysis and Applications*, 19(1), 1-19. <https://doi.org/10.28924/2291-8639-19-2021-1>

Received December, 2021